

2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-

Other names: 3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid
3-(4-hydroxy-3-methoxyphenyl)acrylic acid
3-Methoxy-4-hydroxycinnamic acid
4-Hydroxy-3-methoxycinnamic acid (ferulic acid)
4-hydroxy-3-methoxycinnamic acid
Cinnamic acid, 4-hydroxy-3-methoxy-
coniferic acid
ferulaic acid
ferulic acid

Inchi: InChI=1S/C10H10O4/c1-14-9-6-7(2-4-8(9)11)3-5-10(12)13/h2-6,11H,1H3,(H,12,13)
InchiKey: KSEBMYQBYZTDHS-UHFFFAOYSA-N
Formula: C10H10O4
SMILES: COc1cc(C=CC(=O)O)ccc1O
Mol. weight [g/mol]: 194.18
CAS: 1135-24-6

Physical Properties

Property code	Value	Unit	Source
gf	-309.04	kJ/mol	Joback Method
hf	-481.79	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	79.60	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.499		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	1897.10		NIST Webbook
tb	713.11	K	Joback Method
tc	929.21	K	Joback Method
tf	444.90	K	Solubility of high-value compounds in ethyl lactate: Measurements and modelling
tf	445.90	K	Thermodynamics of a model biological reaction: A comprehensive combined experimental and theoretical study
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.28	J/molxK	929.21	Joback Method
cpg	379.79	J/molxK	749.13	Joback Method
cpg	388.25	J/molxK	785.14	Joback Method
cpg	396.26	J/molxK	821.16	Joback Method
cpg	403.89	J/molxK	857.18	Joback Method
cpg	411.21	J/molxK	893.20	Joback Method
cpg	370.82	J/molxK	713.11	Joback Method
dvisc	0.0000062	Paxs	674.43	Joback Method
dvisc	0.0000104	Paxs	635.75	Joback Method
dvisc	0.0000188	Paxs	597.07	Joback Method
dvisc	0.0000369	Paxs	558.38	Joback Method
dvisc	0.0000802	Paxs	519.70	Joback Method
dvisc	0.0000039	Paxs	713.11	Joback Method
dvisc	0.0001970	Paxs	481.02	Joback Method
hfust	33.34	kJ/mol	444.60	NIST Webbook
hfust	17.89	kJ/mol	435.30	NIST Webbook
hsubt	132.40 ± 1.30	kJ/mol	379.50	NIST Webbook
psub	3.84e-05	kPa	373.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.46e-05	kPa	377.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.96e-05	kPa	377.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	6.46e-05	kPa	377.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	7.97e-05	kPa	379.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	3.88e-05	kPa	373.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.04e-04	kPa	381.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.02e-04	kPa	381.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.00e-04	kPa	381.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.24e-04	kPa	383.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	1.20e-04	kPa	383.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.30e-04	kPa	383.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.56e-04	kPa	385.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.64e-04	kPa	385.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.62e-04	kPa	385.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.96e-04	kPa	387.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.88e-04	kPa	387.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	1.96e-04	kPa	387.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.42e-04	kPa	389.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.35e-04	kPa	389.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.42e-04	kPa	389.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.73e-05	kPa	369.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.26e-05	kPa	369.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.47e-05	kPa	368.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	5.23e-05	kPa	375.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	4.83e-05	kPa	375.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	4.08e-05	kPa	373.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.13e-05	kPa	379.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

Sources

Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method:
 Solubility of high-value compounds in ethyl lactate: Measurements and Modeling Method:
 NIST Webbook:
 Thermodynamics of a model biological reaction: A comprehensive combined experimental and theoretical study: Solubility of Ferulic Acid and Tetramethylpyrazine in Supercritical Carbon Dioxide:
 Crippen Method:
 Temperature and salt addition effects on the solubility behaviour of some phenolics and high-value compounds in environmentally friendly solvents liquid poly(ethylene glycol) and ionic liquids: Experimental study and thermodynamic analysis:

<https://www.doi.org/10.1021/je050293h>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1016/j.jct.2011.12.005>
<http://link.springer.com/article/10.1007/BF02311772>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1135246&Units=SI>
<https://www.doi.org/10.1016/j.fluid.2016.01.035>
<https://www.doi.org/10.1021/je049715y>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
https://www.chemeo.com/doc/models/crippen_log10ws
<https://www.doi.org/10.1016/j.jct.2006.06.014>
<https://www.doi.org/10.1016/j.jct.2013.10.036>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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