

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

Other names:	Cinnamic acid, o-methoxy- o-Methoxycinnamic acid 2-Methoxy-cinnamic acid 3-(2-Methoxyphenyl)-2-propenoic acid (2E)-3-(2-Methoxyphenyl)-2-propenoic acid trans-2-methoxycinnamic acid
Inchi:	InChI=1S/C10H10O3/c1-13-9-5-3-2-4-8(9)6-7-10(11)12/h2-7H,1H3,(H,11,12)
InchiKey:	FEGVSPGUHMGGBO-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	<chem>COc1ccccc1C=CC(=O)O</chem>
Mol. weight [g/mol]:	178.18
CAS:	6099-03-2

Physical Properties

Property code	Value	Unit	Source
chs	-4863.50	kJ/mol	NIST Webbook
gf	-154.42	kJ/mol	Joback Method
hf	-304.48	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.793		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1685.60		NIST Webbook
tb	632.49	K	Joback Method
tc	839.79	K	Joback Method
tf	369.30	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	381.31	J/molxK	839.79	Joback Method
cpg	373.93	J/molxK	805.24	Joback Method
cpg	366.02	J/molxK	770.69	Joback Method
cpg	357.56	J/molxK	736.14	Joback Method
cpg	348.51	J/molxK	701.59	Joback Method
cpg	338.85	J/molxK	667.04	Joback Method
cpg	328.56	J/molxK	632.49	Joback Method
dvisc	0.0023160	Paxs	369.30	Joback Method
dvisc	0.0000563	Paxs	632.49	Joback Method
dvisc	0.0000831	Paxs	588.62	Joback Method
dvisc	0.0001304	Paxs	544.76	Joback Method
dvisc	0.0002217	Paxs	500.89	Joback Method
dvisc	0.0004170	Paxs	457.03	Joback Method
dvisc	0.0008973	Paxs	413.17	Joback Method
hfust	32.54	kJ/mol	458.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6099032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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
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

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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