trans-Ferulic acid

Other names:	(2E)-3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid (E)-3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid (E)-4'-hydroxy-3'-methoxycinnamic acid (E)-4-hydroxy-3-methoxycinnamic acid (E)-ferulic acid 2-propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (E)- 4-Hydroxy-3-methoxycinnamic acid, trans Cinnamic acid, 4-hydroxy-3-methoxy-, trans- Ferulic acid Ferulic acid, trans- cinnamic acid, 4-hydroxy-3-methoxy-, (E)- trans-4-hydroxy-3-methoxycinnamic 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)/b5-3
InchiKey:	KSEBMYQBYZTDHS-HWKANZROSA-N
Formula:	C10H10O4
SMILES:	COc1cc(C=CC(=O)O)ccc1O
Mol. weight [g/mol]:	194.18
CAS:	537-98-4

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	1881.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	713.11	K	Joback Method
tc	929.21	K	Joback Method
tf	481.02	K	Joback Method

vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.82	J/mol×K	713.11	Joback Method
cpg	379.79	J/mol×K	749.13	Joback Method
cpg	388.25	J/mol×K	785.14	Joback Method
cpg	396.26	J/mol×K	821.16	Joback Method
cpg	403.89	J/mol×K	857.18	Joback Method
cpg	411.21	J/mol×K	893.20	Joback Method
cpg	418.28	J/mol×K	929.21	Joback Method
dvisc	0.0001970	Pa×s	481.02	Joback Method
dvisc	0.0000802	Pa×s	519.70	Joback Method
dvisc	0.0000369	Pa×s	558.38	Joback Method
dvisc	0.0000188	Pa×s	597.07	Joback Method
dvisc	0.0000104	Pa×s	635.75	Joback Method
dvisc	0.0000062	Pa×s	674.43	Joback Method
dvisc	0.0000039	Pa×s	713.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Ferulic acid solubility in supercritical carbon dioxide, ethanol and water mixtures:	https://www.doi.org/10.1016/j.jct.2016.08.025
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=C537984&Units=SI

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
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