2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, 2,3-dihydroxypropyl ester, (2E)-

Other names: Glyceryl ferulate
Inchi: InChI=1S/C13H16O6/c1-18-12-6-9(2-4-11(12)16)3-5-13(17)19-8-10(15)7-14/h2-6,10,14-
InchiKey: QXRAHTFDPBQKIM-HWKANZROSA-N
Formula: C13H16O6
SMILES: COc1cc(C=CC(=O)OCC(O)CO)ccc1O
Mol. weight [g/mol]: 268.26
CAS: 120601-69-6

Physical Properties

Property code	Value	Unit	Source
gf	-528.04	kJ/mol	Joback Method
hf	-833.44	kJ/mol	Joback Method
hfus	37.69	kJ/mol	Joback Method
hvap	104.98	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.310		Crippen Method
mcvol	196.890	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	2522.70		NIST Webbook
rinpol	2522.70		NIST Webbook
tb	895.91	K	Joback Method
tc	1104.89	K	Joback Method
tf	582.88	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.68	J/mol×K	895.91	Joback Method
cpg	640.94	J/mol×K	1070.06	Joback Method
cpg	632.75	J/mol×K	1035.23	Joback Method
cpg	624.28	J/mol×K	1000.40	Joback Method
cpg	615.48	J/mol×K	965.57	Joback Method
cpg	606.30	J/mol×K	930.74	Joback Method

cpg	648.92	J/mol×K	1104.89	Joback Method
dvisc	0.0000001	Pa×s	895.91	Joback Method
dvisc	0.0000002	Pa×s	843.74	Joback Method
dvisc	0.0000003	Pa×s	791.57	Joback Method
dvisc	0.0000007	Pa×s	739.39	Joback Method
dvisc	0.0000016	Pa×s	687.22	Joback Method
dvisc	0.0000042	Pa×s	635.05	Joback Method
dvisc	0.0000128	Pa×s	582.88	Joback Method

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=C120601696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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