ethyl (R)-12-hydroxyoleate

Other names: Ethyl ricinoleate
Inchi: InChI=1S/C20H38O3/c1-3-5-6-13-16-19(21)17-14-11-9-7-8-10-12-15-18-20(22)23-4-2/h1
InchiKey: AZXVZUBIFYQWJK-RNUYOQPASA-N
Formula: C20H38O3
SMILES: CCCCCCC(O)CC=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 326.51
CAS: 55066-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-175.44	kJ/mol	Joback Method
hf	-741.22	kJ/mol	Joback Method
hfus	51.11	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.558		Crippen Method
mcvol	301.670	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	829.19	K	Joback Method
tc	1015.59	K	Joback Method
tf	428.06	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	961.68	J/mol×K	829.19	Joback Method
cpg	979.25	J/mol×K	860.26	Joback Method
cpg	995.89	J/mol×K	891.32	Joback Method
cpg	1011.63	J/mol×K	922.39	Joback Method
cpg	1026.51	J/mol×K	953.46	Joback Method
cpg	1040.58	J/mol×K	984.52	Joback Method

cpg	1053.87	J/mol×K	1015.59	Joback Method
dvisc	0.0012401	Pa×s	428.06	Joback Method
dvisc	0.0003197	Pa×s	494.91	Joback Method
dvisc	0.0001138	Pa×s	561.77	Joback Method
dvisc	0.0000505	Pa×s	628.62	Joback Method
dvisc	0.0000262	Pa×s	695.48	Joback Method
dvisc	0.0000152	Pa×s	762.34	Joback Method
dvisc	0.0000097	Pa×s	829.19	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C55066530&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

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