

Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Other names:
(Z,Z,Z)-

2-Monolinolenin

InChI: InChI=1S/C21H36O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-19-20(23)18

InchiKey: GGJRAQULURVTAJ-PDBXOOCHSA-N

Formula: C21H36O4

SMILES: CCC=CCC=CCC=CCCCCCCC(=O)OCC(O)CO

Mol. weight [g/mol]: 352.51

CAS: 55268-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-143.40	kJ/mol	Joback Method
hf	-679.65	kJ/mol	Joback Method
hfus	58.19	kJ/mol	Joback Method
hvap	104.34	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.472		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
tb	952.57	K	Joback Method
tc	1170.58	K	Joback Method
tf	489.99	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.76	J/molxK	952.57	Joback Method
cpg	1051.46	J/molxK	988.90	Joback Method
cpg	1067.35	J/molxK	1025.24	Joback Method
cpg	1082.53	J/molxK	1061.57	Joback Method
cpg	1097.09	J/molxK	1097.91	Joback Method
cpg	1111.13	J/molxK	1134.24	Joback Method

cpg	1124.75	J/molxK	1170.58	Joback Method
dvisc	0.0002781	Paxs	489.99	Joback Method
dvisc	0.0000517	Paxs	567.09	Joback Method
dvisc	0.0000144	Paxs	644.18	Joback Method
dvisc	0.0000053	Paxs	721.28	Joback Method
dvisc	0.0000023	Paxs	798.38	Joback Method
dvisc	0.0000012	Paxs	875.47	Joback Method
dvisc	0.0000007	Paxs	952.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55268581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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