

Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester

Other names:

Aqua Cera
Atlas G 2146
Cerasynt
Cerasynt Special
Clindrol SDG
Diethylene glycol monostearate
Diethylene glycol stearate
Diethylene glycol, monoester with stearic acid
Diglycol monostearate
Diglycol stearate
Emcol CAD
Emcol DS-50 CAD
Emcol ETS
Glyco stearin
Nonex 411
Promul 5080
PEG-2 Stearate
Stearic acid, 2-(2-hydroxyethoxy)ethyl ester
USAF KE-8
NSC 404230
2-(2-hydroxyethoxy)ethyl stearate

Inchi: InChI=1S/C22H44O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22(24)26-21-20-25-19
InchiKey: PWVUXRBUUYZMKM-UHFFFAOYSA-N
Formula: C22H44O4
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCOCCO
Mol. weight [g/mol]: 372.58
CAS: 106-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-341.38	kJ/mol	Joback Method
hf	-1026.66	kJ/mol	Joback Method
hfus	60.80	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.800		Crippen Method

mvol	340.020	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
tb	893.65	K	Joback Method
tc	1098.19	K	Joback Method
tf	492.91	K	Joback Method
vc	1.329	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.44	J/mol×K	893.65	Joback Method
cpg	1227.19	J/mol×K	1064.10	Joback Method
cpg	1212.74	J/mol×K	1030.01	Joback Method
cpg	1197.08	J/mol×K	995.92	Joback Method
cpg	1180.16	J/mol×K	961.83	Joback Method
cpg	1161.96	J/mol×K	927.74	Joback Method
cpg	1240.45	J/mol×K	1098.19	Joback Method
dvisc	0.0000060	Paxs	893.65	Joback Method
dvisc	0.0000091	Paxs	826.86	Joback Method
dvisc	0.0000148	Paxs	760.07	Joback Method
dvisc	0.0000266	Paxs	693.28	Joback Method
dvisc	0.0000538	Paxs	626.49	Joback Method
dvisc	0.0001291	Paxs	559.70	Joback Method
dvisc	0.0003923	Paxs	492.91	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C106116&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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