Hexadecanoic acid, 1,3-propanediyl ester

Other names:	Palmitic acid, trimethylene ester
	1,3-Propanediol dipalmitate
	Hexadecanoic acid, 1,1'-(1,3-propanediyl) ester
Inchi:	InChI=1S/C35H68O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-30-34(36)38-32-29-33-39-
InchiKey:	FBFGIPIHQQUDQF-UHFFFAOYSA-N
Formula:	C35H68O4
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCCOC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	552.91
CAS:	818-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-224.02	kJ/mol	Joback Method
hf	-1255.33	kJ/mol	Joback Method
hfus	91.98	kJ/mol	Joback Method
hvap	111.82	kJ/mol	Joback Method
log10ws	-12.20		Crippen Method
logp	11.426		Crippen Method
mcvol	518.890	ml/mol	McGowan Method
pc	496.91	kPa	Joback Method
tb	1152.78	K	Joback Method
tc	1519.56	K	Joback Method
tf	628.53	K	Joback Method
vc	2.043	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2049.57	J/mol×K	1519.56	Joback Method
cpg	1935.35	J/mol×K	1152.78	Joback Method
cpg	1964.52	J/mol×K	1213.91	Joback Method
cpg	1989.12	J/mol×K	1275.04	Joback Method
cpg	2009.54	J/mol×K	1336.17	Joback Method
cpg	2026.17	J/mol×K	1397.30	Joback Method

cpg	2039.39	J/mol×K	1458.43	Joback Method
dvisc	0.0000050	Pa×s	1152.78	Joback Method
dvisc	0.0001166	Pa×s	628.53	Joback Method
dvisc	0.0000502	Pa×s	715.90	Joback Method
dvisc	0.0000259	Pa×s	803.28	Joback Method
dvisc	0.0000153	Pa×s	890.65	Joback Method
dvisc	0.0000099	Pa×s	978.03	Joback Method
dvisc	0.0000069	Pa×s	1065.40	Joback Method
hfust	133.00	kJ/mol	329.80	NIST Webbook

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=C818213&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
hfust:	Enthalpy of fusion at a given temperature
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