Adipic acid, 8-chloroctyl hexadecyl ester

Inchi: InChI=1S/C30H57ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-14-17-22-27-34-29(32)24-19-20-25-
InchiKey: MGYTWPAMDKJXLU-UHFFFAOYSA-N
Formula: C30H57ClO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 517.22

Physical Properties

Property code	Value	Unit	Source
gf	-278.05	kJ/mol	Joback Method
hf	-1167.87	kJ/mol	Joback Method
hfus	83.23	kJ/mol	Joback Method
hvap	105.07	kJ/mol	Joback Method
log10ws	-10.26		Crippen Method
logp	9.694		Crippen Method
mcvol	460.680	ml/mol	McGowan Method
pc	611.78	kPa	Joback Method
tb	1075.81	K	Joback Method
tc	1360.82	K	Joback Method
tf	602.10	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1633.60	J/mol×K	1075.81	Joback Method
cpg	1656.93	J/mol×K	1123.31	Joback Method
cpg	1677.54	J/mol×K	1170.81	Joback Method
cpg	1695.56	J/mol×K	1218.31	Joback Method
cpg	1711.15	J/mol×K	1265.81	Joback Method
cpg	1724.45	J/mol×K	1313.32	Joback Method
cpg	1735.62	J/mol×K	1360.82	Joback Method
dvisc	0.0001811	Pa×s	602.10	Joback Method
dvisc	0.0000831	Pa×s	681.05	Joback Method
dvisc	0.0000449	Pa×s	760.00	Joback Method

dvisc	0.0000272	Pa×s	838.95	Joback Method
dvisc	0.0000180	Pa×s	917.91	Joback Method
dvisc	0.0000127	Pa×s	996.86	Joback Method
dvisc	0.0000094	Pa×s	1075.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349771&Units=SI
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

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