Adipic acid, 2-chloropropyl heptyl ester

Inchi: InChI=1S/C16H29ClO4/c1-3-4-5-6-9-12-20-15(18)10-7-8-11-16(19)21-13-14(2)17/h14H,
InchiKey: BVAPIZLYVSIXCH-UHFFFAOYSA-N
Formula: C16H29ClO4
SMILES: CCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 320.85

Physical Properties

Property code	Value	Unit	Source
gf	-398.37	kJ/mol	Joback Method
hf	-884.19	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.231		Crippen Method
mcvol	263.420	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2143.00		NIST Webbook
tb	755.05	K	Joback Method
tc	938.27	K	Joback Method
tf	429.32	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.33	J/mol×K	755.05	Joback Method
cpg	781.21	J/mol×K	785.59	Joback Method
cpg	796.21	J/mol×K	816.12	Joback Method
cpg	810.35	J/mol×K	846.66	Joback Method
cpg	823.63	J/mol×K	877.19	Joback Method
cpg	836.07	J/mol×K	907.73	Joback Method
cpg	847.68	J/mol×K	938.27	Joback Method
dvisc	0.0012042	Pa×s	429.32	Joback Method
dvisc	0.0005848	Pa×s	483.61	Joback Method

dvisc	0.0003285	Pa×s	537.90	Joback Method
dvisc	0.0002052	Pa×s	592.18	Joback Method
dvisc	0.0001387	Pa×s	646.47	Joback Method
dvisc	0.0000996	Pa×s	700.76	Joback Method
dvisc	0.0000750	Pa×s	755.05	Joback Method

Sources

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=U353543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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