Adipic acid, 2-chloropropyl octyl ester

Inchi: InChI=1S/C17H31ClO4/c1-3-4-5-6-7-10-13-21-16(19)11-8-9-12-17(20)22-14-15(2)18/h15
InchiKey: XRQJJAULZVTGRQ-UHFFFAOYSA-N
Formula: C17H31ClO4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 334.88

Physical Properties

Property code	Value	Unit	Source
gf	-389.95	kJ/mol	Joback Method
hf	-904.83	kJ/mol	Joback Method
hfus	46.03	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.621		Crippen Method
mcvol	277.510	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2241.00		NIST Webbook
tb	777.93	K	Joback Method
tc	962.16	K	Joback Method
tf	440.59	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.99	J/mol×K	777.93	Joback Method
cpg	839.25	J/mol×K	808.63	Joback Method
cpg	854.58	J/mol×K	839.34	Joback Method
cpg	869.00	J/mol×K	870.04	Joback Method
cpg	882.53	J/mol×K	900.75	Joback Method
cpg	895.16	J/mol×K	931.45	Joback Method
cpg	906.92	J/mol×K	962.16	Joback Method
dvisc	0.0010819	Pa×s	440.59	Joback Method
dvisc	0.0005194	Pa×s	496.81	Joback Method

dvisc	0.0002895	Pa×s	553.04	Joback Method
dvisc	0.0001797	Pa×s	609.26	Joback Method
dvisc	0.0001209	Pa×s	665.48	Joback Method
dvisc	0.0000866	Pa×s	721.71	Joback Method
dvisc	0.0000650	Pa×s	777.93	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353544&Units=SI

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