Sebacic acid, 2-chloropropyl isohexyl ester

Inchi: InChI=1S/C19H35ClO4/c1-16(2)11-10-14-23-18(21)12-8-6-4-5-7-9-13-19(22)24-15-17(3)
InchiKey: SEKIWLWMCBKNDZ-UHFFFAOYSA-N
Formula: C19H35ClO4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 362.93

Physical Properties

Property code	Value	Unit	Source
gf	-375.55	kJ/mol	Joback Method
hf	-951.39	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	79.81	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.257		Crippen Method
mcvol	305.690	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2445.00		NIST Webbook
tb	823.25	K	Joback Method
tc	1012.43	K	Joback Method
tf	448.13	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.55	J/mol×K	823.25	Joback Method
cpg	1016.57	J/mol×K	980.90	Joback Method
cpg	1003.62	J/mol×K	949.37	Joback Method
cpg	989.65	J/mol×K	917.84	Joback Method
cpg	974.66	J/mol×K	886.31	Joback Method
cpg	958.63	J/mol×K	854.78	Joback Method
cpg	1028.54	J/mol×K	1012.43	Joback Method
dvisc	0.0000445	Pa×s	823.25	Joback Method
dvisc	0.0000605	Pa×s	760.73	Joback Method

dvisc	0.0000870	Pa×s	698.21	Joback Method
dvisc	0.0001344	Pa×s	635.69	Joback Method
dvisc	0.0002281	Pa×s	573.17	Joback Method
dvisc	0.0004406	Pa×s	510.65	Joback Method
dvisc	0.0010229	Pa×s	448.13	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=U355445&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