Sebacic acid, 2-chloropropyl isobutyl ester

Inchi: InChI=1S/C17H31ClO4/c1-14(2)12-21-16(19)10-8-6-4-5-7-9-11-17(20)22-13-15(3)18/h14
InchiKey: XJHDWUFLKOULST-UHFFFAOYSA-N
Formula: C17H31ClO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 334.88

Physical Properties

Property code	Value	Unit	Source
gf	-392.39	kJ/mol	Joback Method
hf	-910.11	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.477		Crippen Method
mcvol	277.510	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	777.49	K	Joback Method
tc	963.26	K	Joback Method
tf	425.59	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.50	J/mol×K	777.49	Joback Method
cpg	839.90	J/mol×K	808.45	Joback Method
cpg	855.35	J/mol×K	839.41	Joback Method
cpg	869.87	J/mol×K	870.38	Joback Method
cpg	883.46	J/mol×K	901.34	Joback Method
cpg	896.14	J/mol×K	932.30	Joback Method
cpg	907.93	J/mol×K	963.26	Joback Method
dvisc	0.0012997	Pa×s	425.59	Joback Method

dvisc	0.0005702	Pa×s	484.24	Joback Method
dvisc	0.0002990	Pa×s	542.89	Joback Method
dvisc	0.0001778	Pa×s	601.54	Joback Method
dvisc	0.0001159	Pa×s	660.19	Joback Method
dvisc	0.0000811	Pa×s	718.84	Joback Method
dvisc	0.0000598	Pa×s	777.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355443&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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