

Sebacic acid, 2-chloropropyl isoheptyl 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)CCCCCCCC(=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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.55	J/molxK	823.25	Joback Method
cpg	958.63	J/molxK	854.78	Joback Method
cpg	974.66	J/molxK	886.31	Joback Method
cpg	989.65	J/molxK	917.84	Joback Method
cpg	1003.62	J/molxK	949.37	Joback Method
cpg	1016.57	J/molxK	980.90	Joback Method
cpg	1028.54	J/molxK	1012.43	Joback Method
dvisc	0.0010229	Paxs	448.13	Joback Method
dvisc	0.0004406	Paxs	510.65	Joback Method

dvisc	0.0002281	Paxs	573.17	Joback Method
dvisc	0.0001344	Paxs	635.69	Joback Method
dvisc	0.0000870	Paxs	698.21	Joback Method
dvisc	0.0000605	Paxs	760.73	Joback Method
dvisc	0.0000445	Paxs	823.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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