

Sebacic acid, 2-chloropropyl hexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-373.11	kJ/mol	Joback Method
hf	-946.11	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.401		Crippen Method
mcvol	305.690	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpola	2480.00		NIST Webbook
tb	823.69	K	Joback Method
tc	1011.93	K	Joback Method
tf	463.13	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.05	J/molxK	823.69	Joback Method
cpg	1015.87	J/molxK	980.56	Joback Method
cpg	1002.91	J/molxK	949.19	Joback Method
cpg	988.97	J/molxK	917.81	Joback Method
cpg	974.02	J/molxK	886.44	Joback Method
cpg	958.06	J/molxK	855.06	Joback Method
cpg	1027.85	J/molxK	1011.93	Joback Method
dvisc	0.0000485	Paxs	823.69	Joback Method
dvisc	0.0000649	Paxs	763.60	Joback Method

dvisc	0.0000912	Paxs	703.50	Joback Method
dvisc	0.0001367	Paxs	643.41	Joback Method
dvisc	0.0002226	Paxs	583.32	Joback Method
dvisc	0.0004054	Paxs	523.22	Joback Method
dvisc	0.0008626	Paxs	463.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355446&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

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