

Sebacic acid, 2,2-dichloroethyl heptyl ester

Inchi:	InChI=1S/C19H34Cl2O4/c1-2-3-4-9-12-15-24-18(22)13-10-7-5-6-8-11-14-19(23)25-16-17
InchiKey:	QLJZMZLGDQEOIW-UHFFFAOYSA-N
Formula:	C19H34Cl2O4
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	397.38

Physical Properties

Property code	Value	Unit	Source
gf	-385.04	kJ/mol	Joback Method
hf	-961.85	kJ/mol	Joback Method
hfus	55.41	kJ/mol	Joback Method
hvap	84.58	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.968		Crippen Method
mvol	317.930	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rmpol	2635.00		NIST Webbook
tb	861.12	K	Joback Method
tc	1056.11	K	Joback Method
tf	493.05	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.57	J/molxK	861.12	Joback Method
cpg	1040.18	J/molxK	1023.61	Joback Method
cpg	1028.34	J/molxK	991.11	Joback Method
cpg	1015.48	J/molxK	958.61	Joback Method
cpg	1001.58	J/molxK	926.12	Joback Method
cpg	986.62	J/molxK	893.62	Joback Method
cpg	1051.01	J/molxK	1056.11	Joback Method
dvisc	0.0000411	Paxs	861.12	Joback Method
dvisc	0.0000548	Paxs	799.77	Joback Method

dvisc	0.0000765	Paxs	738.43	Joback Method
dvisc	0.0001135	Paxs	677.09	Joback Method
dvisc	0.0001822	Paxs	615.74	Joback Method
dvisc	0.0003248	Paxs	554.39	Joback Method
dvisc	0.0006685	Paxs	493.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355471&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

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
mccvol:	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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