

Sebacic acid, 2,2-dichloroethyl pentyl ester

Inchi:	InChI=1S/C17H30Cl2O4/c1-2-3-10-13-22-16(20)11-8-6-4-5-7-9-12-17(21)23-14-15(18)19
InchiKey:	PQNPDDVBZYKSF-UHFFFAOYSA-N
Formula:	C17H30Cl2O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	369.32

Physical Properties

Property code	Value	Unit	Source
gf	-401.88	kJ/mol	Joback Method
hf	-920.57	kJ/mol	Joback Method
hfus	50.23	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.188		Crippen Method
mvol	289.750	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	815.36	K	Joback Method
tc	1005.28	K	Joback Method
tf	470.51	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.42	J/molxK	815.36	Joback Method
cpg	919.55	J/molxK	973.63	Joback Method
cpg	907.98	J/molxK	941.97	Joback Method
cpg	895.51	J/molxK	910.32	Joback Method
cpg	882.10	J/molxK	878.67	Joback Method
cpg	867.74	J/molxK	847.01	Joback Method
cpg	930.21	J/molxK	1005.28	Joback Method
dvisc	0.0000557	Paxs	815.36	Joback Method

dvisc	0.0000738	Paxs	757.88	Joback Method
dvisc	0.0001025	Paxs	700.41	Joback Method
dvisc	0.0001508	Paxs	642.93	Joback Method
dvisc	0.0002395	Paxs	585.46	Joback Method
dvisc	0.0004205	Paxs	527.99	Joback Method
dvisc	0.0008474	Paxs	470.51	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=U355469&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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