

Sebacic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C16H28Cl2O4/c1-13(2)11-21-15(19)9-7-5-3-4-6-8-10-16(20)22-12-14(17)18/h
InchiKey:	SHRBYULMOKRDLC-UHFFFAOYSA-N
Formula:	C16H28Cl2O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	355.30

Physical Properties

Property code	Value	Unit	Source
gf	-412.74	kJ/mol	Joback Method
hf	-905.21	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.653		Crippen Method
mvol	275.660	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	792.04	K	Joback Method
tc	982.16	K	Joback Method
tf	444.24	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.14	J/molxK	792.04	Joback Method
cpg	810.22	J/molxK	823.73	Joback Method
cpg	824.37	J/molxK	855.41	Joback Method
cpg	837.60	J/molxK	887.10	Joback Method
cpg	849.92	J/molxK	918.79	Joback Method
cpg	861.34	J/molxK	950.48	Joback Method
cpg	871.89	J/molxK	982.16	Joback Method
dvisc	0.0011212	Paxs	444.24	Joback Method

dvisc	0.0005180	Paxs	502.21	Joback Method
dvisc	0.0002808	Paxs	560.17	Joback Method
dvisc	0.0001707	Paxs	618.14	Joback Method
dvisc	0.0001131	Paxs	676.11	Joback Method
dvisc	0.0000799	Paxs	734.07	Joback Method
dvisc	0.0000594	Paxs	792.04	Joback Method

Sources

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=U355467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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