

Sebacic acid, 2,2-dichloroethyl ethyl ester

Inchi:	InChI=1S/C14H24Cl2O4/c1-2-19-13(17)9-7-5-3-4-6-8-10-14(18)20-11-12(15)16/h12H,2-
InchiKey:	BVCZMWSVTSHPBUM-UHFFFAOYSA-N
Formula:	C14H24Cl2O4
SMILES:	CCOC(=O)CCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	327.24

Physical Properties

Property code	Value	Unit	Source
gf	-427.14	kJ/mol	Joback Method
hf	-858.65	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.017		Crippen Method
mcvol	247.480	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinsol	2134.00		NIST Webbook
tb	746.72	K	Joback Method
tc	934.24	K	Joback Method
tf	436.70	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.87	J/molxK	746.72	Joback Method
cpg	696.04	J/molxK	777.97	Joback Method
cpg	709.39	J/molxK	809.23	Joback Method
cpg	721.94	J/molxK	840.48	Joback Method
cpg	733.69	J/molxK	871.74	Joback Method
cpg	744.64	J/molxK	902.99	Joback Method
cpg	754.82	J/molxK	934.24	Joback Method
dvisc	0.0011757	Paxs	436.70	Joback Method
dvisc	0.0006045	Paxs	488.37	Joback Method

dvisc	0.0003530	Paxs	540.04	Joback Method
dvisc	0.0002264	Paxs	591.71	Joback Method
dvisc	0.0001560	Paxs	643.38	Joback Method
dvisc	0.0001136	Paxs	695.05	Joback Method
dvisc	0.0000864	Paxs	746.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355465&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
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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