

Glutaric acid, cyclohexylmethyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C14H22Cl2O4/c15-12(16)10-20-14(18)8-4-7-13(17)19-9-11-5-2-1-3-6-11/h11-
InchiKey:	WRUXCTAQXJZPNZ-UHFFFAOYSA-N
Formula:	C14H22Cl2O4
SMILES:	O=C(CCCC(=O)OCC1CCCCC1)OCC(Cl)Cl
Mol. weight [g/mol]:	325.23

Physical Properties

Property code	Value	Unit	Source
gf	-402.69	kJ/mol	Joback Method
hf	-804.33	kJ/mol	Joback Method
hfus	34.30	kJ/mol	Joback Method
hvap	73.88	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.627		Crippen Method
mvol	236.620	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2171.00		NIST Webbook
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tb	766.27	K	Joback Method
tc	976.34	K	Joback Method
tf	444.08	K	Joback Method
vc	0.892	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.53	J/molxK	766.27	Joback Method
cpg	691.22	J/molxK	801.28	Joback Method
cpg	705.76	J/molxK	836.29	Joback Method
cpg	719.15	J/molxK	871.31	Joback Method
cpg	731.42	J/molxK	906.32	Joback Method
cpg	742.57	J/molxK	941.33	Joback Method
cpg	752.62	J/molxK	976.34	Joback Method
dvisc	0.0013580	Paxs	444.08	Joback Method

dvisc	0.0006763	Paxs	497.78	Joback Method
dvisc	0.0003858	Paxs	551.48	Joback Method
dvisc	0.0002431	Paxs	605.17	Joback Method
dvisc	0.0001652	Paxs	658.87	Joback Method
dvisc	0.0001189	Paxs	712.57	Joback Method
dvisc	0.0000897	Paxs	766.27	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=U393540&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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