Glutaric acid, 1-cyclopentylethyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H22Cl2O4/c1-10(11-5-2-3-6-11)20-14(18)8-4-7-13(17)19-9-12(15)16/h10-1

InchiKey: SAQLFYZZSWNROD-UHFFFAOYSA-N

Formula: C14H22Cl2O4

SMILES: CC(OC(=O)CCCC(=O)OCC(Cl)Cl)C1CCCC1

Mol. weight [g/mol]: 325.23

Physical Properties

Property code	Value	Unit	Source
gf	-393.03	kJ/mol	Joback Method
hf	-803.45	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.626		Crippen Method
mcvol	236.620	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	761.56	K	Joback Method
tc	969.64	K	Joback Method
tf	432.60	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.81	J/mol×K	761.56	Joback Method
cpg	688.22	J/mol×K	796.24	Joback Method
cpg	702.56	J/mol×K	830.92	Joback Method
cpg	715.82	J/mol×K	865.60	Joback Method
cpg	728.04	J/mol×K	900.28	Joback Method
cpg	739.24	J/mol×K	934.96	Joback Method
cpg	749.43	J/mol×K	969.64	Joback Method
dvisc	0.0017104	Pa×s	432.60	Joback Method

dvisc	0.0008489	Pa×s	487.43	Joback Method
dvisc	0.0004854	Pa×s	542.25	Joback Method
dvisc	0.0003076	Pa×s	597.08	Joback Method
dvisc	0.0002104	Pa×s	651.91	Joback Method
dvisc	0.0001527	Pa×s	706.73	Joback Method
dvisc	0.0001161	Pa×s	761.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U405461&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