Glutaric acid, 2,2-dichloroethyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C13H22Cl2O4/c1-4-10(9(2)3)19-13(17)7-5-6-12(16)18-8-11(14)15/h9-11H,4-8

InchiKey: QBQMHLRJWHGJRL-UHFFFAOYSA-N

Formula: C13H22Cl2O4

SMILES: CCC(OC(=O)CCCC(=O)OCC(Cl)Cl)C(C)C

Mol. weight [g/mol]: 313.22

Physical Properties

Property code	Value	Unit	Source
gf	-440.44	kJ/mol	Joback Method
hf	-848.57	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.481		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
tb	722.96	K	Joback Method
tc	915.97	K	Joback Method
tf	395.43	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.19	J/mol×K	722.96	Joback Method
cpg	690.64	J/mol×K	883.80	Joback Method
cpg	679.79	J/mol×K	851.63	Joback Method
cpg	668.12	J/mol×K	819.47	Joback Method
cpg	655.64	J/mol×K	787.30	Joback Method
cpg	642.33	J/mol×K	755.13	Joback Method
cpg	700.70	J/mol×K	915.97	Joback Method
dvisc	0.0000849	Pa×s	722.96	Joback Method

dvisc	0.0001156	Pa×s	668.37	Joback Method
dvisc	0.0001661	Pa×s	613.78	Joback Method
dvisc	0.0002563	Pa×s	559.20	Joback Method
dvisc	0.0004344	Pa×s	504.61	Joback Method
dvisc	0.0008368	Pa×s	450.02	Joback Method
dvisc	0.0019317	Pa×s	395.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393495&Units=SI
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

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