Glutaric acid, 2,2-dichloroethyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C14H24Cl2O5/c1-11(6-8-19-2)7-9-20-13(17)4-3-5-14(18)21-10-12(15)16/h11-1

InchiKey: VIJJAZRSZPYWHA-UHFFFAOYSA-N

Formula: C14H24Cl2O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 343.24

Physical Properties

Property code	Value	Unit	Source
gf	-534.58	kJ/mol	Joback Method
hf	-996.15	kJ/mol	Joback Method
hfus	40.13	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.109		Crippen Method
mcvol	253.350	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2146.00		NIST Webbook
tb	768.70	K	Joback Method
tc	958.84	K	Joback Method
tf	443.93	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.29	J/mol×K	768.70	Joback Method
cpg	771.88	J/mol×K	927.15	Joback Method
cpg	761.33	J/mol×K	895.46	Joback Method
cpg	749.90	J/mol×K	863.77	Joback Method
cpg	737.58	J/mol×K	832.08	Joback Method
cpg	724.37	J/mol×K	800.39	Joback Method
cpg	781.54	J/mol×K	958.84	Joback Method
dvisc	0.0000597	Pa×s	768.70	Joback Method

dvisc	0.0000795	Pa×s	714.57	Joback Method
dvisc	0.0001110	Pa×s	660.44	Joback Method
dvisc	0.0001644	Pa×s	606.32	Joback Method
dvisc	0.0002630	Pa×s	552.19	Joback Method
dvisc	0.0004658	Pa×s	498.06	Joback Method
dvisc	0.0009488	Pa×s	443.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393521&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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