Glutaric acid, (2-chlorocyclohexyl)methyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H21Cl3O4/c15-11-5-2-1-4-10(11)8-20-13(18)6-3-7-14(19)21-9-12(16)17/h1

InchiKey: NHIGIWVVKZYBCS-UHFFFAOYSA-N

Formula: C14H21Cl3O4

SMILES: O=C(CCCC(=O)OCC1CCCCC1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 359.67

Physical Properties

Property code	Value	Unit	Source
gf	-422.33	kJ/mol	Joback Method
hf	-840.41	kJ/mol	Joback Method
hfus	39.56	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.844		Crippen Method
mcvol	248.860	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	799.03	K	Joback Method
tc	1012.43	K	Joback Method
tf	469.76	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.89	J/mol×K	799.03	Joback Method
cpg	720.68	J/mol×K	834.60	Joback Method
cpg	734.27	J/mol×K	870.16	Joback Method
cpg	746.65	J/mol×K	905.73	Joback Method
cpg	757.84	J/mol×K	941.30	Joback Method
cpg	767.85	J/mol×K	976.87	Joback Method
cpg	776.68	J/mol×K	1012.43	Joback Method
dvisc	0.0011341	Pa×s	469.76	Joback Method

dvisc	0.0006088	Pa×s	524.64	Joback Method
dvisc	0.0003677	Pa×s	579.52	Joback Method
dvisc	0.0002423	Pa×s	634.39	Joback Method
dvisc	0.0001707	Pa×s	689.27	Joback Method
dvisc	0.0001266	Pa×s	744.15	Joback Method
dvisc	0.0000978	Pa×s	799.03	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=U405444&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