Glutaric acid, 2,2-dichloroethyl 2-methoxyphenyl ester

Inchi: InChI=1S/C14H16Cl2O5/c1-19-10-5-2-3-6-11(10)21-14(18)8-4-7-13(17)20-9-12(15)16/h2

InchiKey: FKODKESYZVUPSG-UHFFFAOYSA-N

Formula: C14H16Cl2O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 335.18

Physical Properties

Property code	Value	Unit	Source
gf	-429.36	kJ/mol	Joback Method
hf	-765.81	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.118		Crippen Method
mcvol	229.590	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	800.80	K	Joback Method
tc	1015.32	K	Joback Method
tf	497.87	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.65	J/mol×K	800.80	Joback Method
cpg	666.58	J/mol×K	979.57	Joback Method
cpg	658.64	J/mol×K	943.81	Joback Method
cpg	649.67	J/mol×K	908.06	Joback Method
cpg	639.69	J/mol×K	872.31	Joback Method
cpg	628.68	J/mol×K	836.55	Joback Method
cpg	673.49	J/mol×K	1015.32	Joback Method
dvisc	0.0000660	Pa×s	800.80	Joback Method

dvisc	0.0000838	Pa×s	750.31	Joback Method
dvisc	0.0001102	Pa×s	699.82	Joback Method
dvisc	0.0001513	Pa×s	649.34	Joback Method
dvisc	0.0002190	Pa×s	598.85	Joback Method
dvisc	0.0003395	Pa×s	548.36	Joback Method
dvisc	0.0005751	Pa×s	497.87	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=U391757&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