Glutaric acid, 2,2-dichloroethyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C14H15Cl3O5/c1-20-11-7-9(15)5-6-10(11)22-14(19)4-2-3-13(18)21-8-12(16)17

InchiKey: XSDKLDUDSXYTFN-UHFFFAOYSA-N

Formula: C14H15Cl3O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 369.62

Physical Properties

Property code	Value	Unit	Source
gf	-450.92	kJ/mol	Joback Method
hf	-793.02	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	83.85	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.771		Crippen Method
mcvol	241.830	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	843.21	K	Joback Method
tc	1061.97	K	Joback Method
tf	540.31	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.19	J/mol×K	843.21	Joback Method
cpg	680.32	J/mol×K	1025.51	Joback Method
cpg	673.82	J/mol×K	989.05	Joback Method
cpg	666.25	J/mol×K	952.59	Joback Method
cpg	657.62	J/mol×K	916.13	Joback Method
cpg	647.93	J/mol×K	879.67	Joback Method
cpg	685.74	J/mol×K	1061.97	Joback Method
dvisc	0.0000574	Pa×s	843.21	Joback Method

dvisc	0.0000719	Pa×s	792.73	Joback Method
dvisc	0.0000927	Pa×s	742.24	Joback Method
dvisc	0.0001241	Pa×s	691.76	Joback Method
dvisc	0.0001741	Pa×s	641.28	Joback Method
dvisc	0.0002586	Pa×s	590.79	Joback Method
dvisc	0.0004136	Pa×s	540.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393906&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