Glutaric acid, 2,2-dichloroethyl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C14H15Cl3O4/c1-9-5-6-10(15)11(7-9)21-14(19)4-2-3-13(18)20-8-12(16)17/h5-

InchiKey: OUDHCKOTGASFBB-UHFFFAOYSA-N

Formula: C14H15Cl3O4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCC(=O)OCC(Cl)Cl)c1

Mol. weight [g/mol]: 353.62

Physical Properties

Property code	Value	Unit	Source
gf	-345.92	kJ/mol	Joback Method
hf	-660.80	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.071		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	820.79	K	Joback Method
tc	1040.75	K	Joback Method
tf	518.08	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/mol×K	820.79	Joback Method
cpg	623.13	J/mol×K	857.45	Joback Method
cpg	633.33	J/mol×K	894.11	Joback Method
cpg	642.56	J/mol×K	930.77	Joback Method
cpg	650.83	J/mol×K	967.43	Joback Method
cpg	658.15	J/mol×K	1004.09	Joback Method
cpg	664.54	J/mol×K	1040.75	Joback Method
dvisc	0.0005822	Pa×s	518.08	Joback Method

dvisc	0.0003575	Pa×s	568.53	Joback Method
dvisc	0.0002376	Pa×s	618.98	Joback Method
dvisc	0.0001680	Pa×s	669.43	Joback Method
dvisc	0.0001247	Pa×s	719.89	Joback Method
dvisc	0.0000962	Pa×s	770.34	Joback Method
dvisc	0.0000767	Pa×s	820.79	Joback Method

Sources

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=U393420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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