Glutaric acid, 2,2-dichloroethyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C13H11Cl5O4/c14-7-4-9(16)10(5-8(7)15)22-13(20)3-1-2-12(19)21-6-11(17)18/

InchiKey: LSFWTKYGIGZMPJ-UHFFFAOYSA-N

Formula: C13H11Cl5O4

SMILES: O=C(CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 408.49

Physical Properties

Property code	Value	Unit	Source
gf	-387.83	kJ/mol	Joback Method
hf	-683.11	kJ/mol	Joback Method
hfus	45.34	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.069		Crippen Method
mcvol	246.350	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	877.75	K	Joback Method
tc	1107.09	K	Joback Method
tf	579.17	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.61	J/mol×K	877.75	Joback Method
cpg	604.07	J/mol×K	915.97	Joback Method
cpg	611.57	J/mol×K	954.20	Joback Method
cpg	618.11	J/mol×K	992.42	Joback Method
cpg	623.70	J/mol×K	1030.64	Joback Method
cpg	628.34	J/mol×K	1068.87	Joback Method
cpg	632.03	J/mol×K	1107.09	Joback Method
dvisc	0.0003942	Pa×s	579.17	Joback Method

dvisc	0.0002600	Pa×s	628.93	Joback Method
dvisc	0.0001823	Pa×s	678.70	Joback Method
dvisc	0.0001342	Pa×s	728.46	Joback Method
dvisc	0.0001027	Pa×s	778.22	Joback Method
dvisc	0.0000812	Pa×s	827.99	Joback Method
dvisc	0.0000659	Pa×s	877.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392160&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