Glutaric acid, 2,2-dichloroethyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C13H12Cl3FO4/c14-8-3-1-4-9(17)13(8)21-12(19)6-2-5-11(18)20-7-10(15)16/h1

InchiKey: QNWGBIJXOYWTRX-UHFFFAOYSA-N

Formula: C13H12Cl3FO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 357.59

Physical Properties

Property code	Value	Unit	Source
gf	-549.15	kJ/mol	Joback Method
hf	-836.27	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	78.39	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.902		Crippen Method
mcvol	223.640	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	797.18	K	Joback Method
tc	1012.12	K	Joback Method
tf	507.40	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.86	J/mol×K	797.18	Joback Method
cpg	576.20	J/mol×K	833.00	Joback Method
cpg	585.65	J/mol×K	868.83	Joback Method
cpg	594.23	J/mol×K	904.65	Joback Method
cpg	601.95	J/mol×K	940.47	Joback Method
cpg	608.80	J/mol×K	976.30	Joback Method
cpg	614.80	J/mol×K	1012.12	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=U391582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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