Glutaric acid, 2,2-dichloroethyl 3-fluorophenyl ester

Inchi: InChI=1S/C13H13Cl2FO4/c14-11(15)8-19-12(17)5-2-6-13(18)20-10-4-1-3-9(16)7-10/h1,3

InchiKey: RBVOOMBGJLLALY-UHFFFAOYSA-N

Formula: C13H13Cl2FO4

SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)OCC(Cl)Cl

Mol. weight [g/mol]: 323.14

Physical Properties

Property code	Value	Unit	Source
gf	-527.59	kJ/mol	Joback Method
hf	-809.06	kJ/mol	Joback Method
hfus	36.60	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.248		Crippen Method
mcvol	211.400	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	754.77	K	Joback Method
tc	965.56	K	Joback Method
tf	464.96	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.34	J/mol×K	754.77	Joback Method
cpg	556.83	J/mol×K	789.90	Joback Method
cpg	567.45	J/mol×K	825.03	Joback Method
cpg	577.20	J/mol×K	860.17	Joback Method
cpg	586.09	J/mol×K	895.30	Joback Method
cpg	594.15	J/mol×K	930.43	Joback Method
cpg	601.36	J/mol×K	965.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392090&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
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