Glutaric acid, (2-chlorocyclohexyl)methyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H21Cl2FO4/c19-13-6-2-1-5-12(13)11-24-16(22)9-4-10-17(23)25-18-14(20)7-3-8-15(18)21/h3,7-8,12-13H,1-2,4-6,9-11H2

InchiKey: XZWZUNDAQLFIQZ-UHFFFAOYSA-N

Formula: C18H21Cl2FO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCC1CCCCC1Cl

Mol. weight [g/mol]: 391.26

Physical Properties

Property code	Value	Unit	Source
gf	-475.94	kJ/mol	Joback Method
hf	-884.47	kJ/mol	Joback Method
hfus	45.59	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.896		Crippen Method
mcvol	270.990	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	889.47	K	Joback Method
tc	1113.18	K	Joback Method
tf	551.97	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.54	J/mol×K	889.47	Joback Method
cpg	831.17	J/mol×K	926.75	Joback Method
cpg	843.35	J/mol×K	964.04	Joback Method
cpg	854.10	J/mol×K	1001.32	Joback Method
cpg	863.44	J/mol×K	1038.61	Joback Method
cpg	871.39	J/mol×K	1075.89	Joback Method
cpg	877.96	J/mol×K	1113.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405449&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