Glutaric acid, (cyclohex-3-enyl)methyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H20ClFO4/c19-14-8-4-9-15(20)18(14)24-17(22)11-5-10-16(21)23-12-13-6-

InchiKey: BCBOMPUHYDLQCB-UHFFFAOYSA-N

Formula: C18H20ClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCC1CC=CCC1

Mol. weight [g/mol]: 354.80

Physical Properties

Property code	Value	Unit	Source
gf	-426.34	kJ/mol	Joback Method
hf	-790.61	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	81.86	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.454		Crippen Method
mcvol	254.450	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	855.87	K	Joback Method
tc	1077.34	K	Joback Method
tf	527.05	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.24	J/mol×K	855.87	Joback Method
cpg	774.25	J/mol×K	892.78	Joback Method
cpg	786.93	J/mol×K	929.69	Joback Method
cpg	798.31	J/mol×K	966.61	Joback Method
cpg	808.42	J/mol×K	1003.52	Joback Method
cpg	817.28	J/mol×K	1040.43	Joback Method
cpg	824.91	J/mol×K	1077.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405530&Units=SI

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