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

Inchi: InChI=1S/C18H22ClFO4/c19-14-7-2-1-6-13(14)12-23-17(21)10-5-11-18(22)24-16-9-4-3-8

InchiKey: IVHMXXZBGHBESZ-UHFFFAOYSA-N

Formula: C18H22ClFO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCC1CCCCC1Cl

Mol. weight [g/mol]: 356.82

Physical Properties

Property code	Value	Unit	Source
gf	-454.38	kJ/mol	Joback Method
hf	-857.26	kJ/mol	Joback Method
hfus	41.78	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.242		Crippen Method
mcvol	258.750	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	847.06	K	Joback Method
tc	1066.37	K	Joback Method
tf	509.53	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.91	J/mol×K	847.06	Joback Method
cpg	809.20	J/mol×K	883.61	Joback Method
cpg	823.07	J/mol×K	920.16	Joback Method
cpg	835.53	J/mol×K	956.72	Joback Method
cpg	846.62	J/mol×K	993.27	Joback Method
cpg	856.35	J/mol×K	1029.82	Joback Method
cpg	864.74	J/mol×K	1066.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405446&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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