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

Inchi: InChI=1S/C19H26ClFO4/c1-2-3-4-5-6-7-14-24-17(22)12-9-13-18(23)25-19-15(20)10-8-11

InchiKey: RBBPXOIEBVYLLG-UHFFFAOYSA-N

Formula: C19H26ClFO4

SMILES: CCCCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 372.86

Physical Properties

Property code	Value	Unit	Source
gf	-472.33	kJ/mol	Joback Method
hf	-923.35	kJ/mol	Joback Method
hfus	51.08	kJ/mol	Joback Method
hvap	83.37	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.458		Crippen Method
mcvol	283.700	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	860.04	K	Joback Method
tc	1061.39	K	Joback Method
tf	530.18	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.73	J/mol×K	860.04	Joback Method
cpg	867.03	J/mol×K	893.60	Joback Method
cpg	880.25	J/mol×K	927.16	Joback Method
cpg	892.41	J/mol×K	960.72	Joback Method
cpg	903.53	J/mol×K	994.28	Joback Method
cpg	913.64	J/mol×K	1027.83	Joback Method
cpg	922.74	J/mol×K	1061.39	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=U391510&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