Glutaric acid, 2-chloro-6-fluorophenyl 3-octyl ester

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

InchiKey: HAPSBMKWZZEASR-UHFFFAOYSA-N

Formula: C19H26ClFO4

SMILES: CCCCCC(CC)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 372.86

Physical Properties

Property code	Value	Unit	Source
gf	-474.77	kJ/mol	Joback Method
hf	-928.63	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	82.98	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.457		Crippen Method
mcvol	283.700	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	859.60	K	Joback Method
tc	1062.46	K	Joback Method
tf	515.18	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.27	J/mol×K	859.60	Joback Method
cpg	867.65	J/mol×K	893.41	Joback Method
cpg	880.93	J/mol×K	927.22	Joback Method
cpg	893.13	J/mol×K	961.03	Joback Method
cpg	904.26	J/mol×K	994.84	Joback Method
cpg	914.35	J/mol×K	1028.65	Joback Method
cpg	923.41	J/mol×K	1062.46	Joback Method

Sources

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=U391565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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