Glutaric acid, 3-chlorophenyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C18H13ClF4O4/c19-11-4-1-5-12(10-11)26-15(24)8-3-9-16(25)27-14-7-2-6-13(1

InchiKey: MIVGWFDHQGOVDN-UHFFFAOYSA-N

Formula: C18H13ClF4O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 404.74

Physical Properties

Property code	Value	Unit	Source
gf	-959.56	kJ/mol	Joback Method
hf	-1274.73	kJ/mol	Joback Method
hfus	43.97	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.179		Crippen Method
mcvol	251.160	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	863.40	K	Joback Method
tc	1077.89	K	Joback Method
tf	562.04	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.30	J/mol×K	863.40	Joback Method
cpg	730.00	J/mol×K	899.15	Joback Method
cpg	739.69	J/mol×K	934.90	Joback Method
cpg	748.40	J/mol×K	970.65	Joback Method
cpg	756.18	J/mol×K	1006.40	Joback Method
cpg	763.07	J/mol×K	1042.15	Joback Method
cpg	769.12	J/mol×K	1077.89	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=U393624&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