Glutaric acid, 2-chloro-6-fluorophenyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C18H12ClF5O4/c19-11-5-2-6-12(20)17(11)28-15(26)9-3-8-14(25)27-13-7-1-4-1

InchiKey: QRCWAUHDXOSWMY-UHFFFAOYSA-N

Formula: C18H12ClF5O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 422.73

Physical Properties

Property code	Value	Unit	Source
gf	-1164.00	kJ/mol	Joback Method
hf	-1482.31	kJ/mol	Joback Method
hfus	46.66	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.318		Crippen Method
mcvol	252.930	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	867.65	K	Joback Method
tc	1077.78	K	Joback Method
tf	575.15	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.15	J/mol×K	867.65	Joback Method
cpg	735.40	J/mol×K	902.67	Joback Method
cpg	744.68	J/mol×K	937.69	Joback Method
cpg	753.02	J/mol×K	972.72	Joback Method
cpg	760.45	J/mol×K	1007.74	Joback Method
cpg	767.01	J/mol×K	1042.76	Joback Method
cpg	772.74	J/mol×K	1077.78	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=U393623&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