Glutaric acid, 2-chloro-6-fluorophenyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H15ClF2O5/c1-24-15-10-11(20)8-9-14(15)25-16(22)6-3-7-17(23)26-18-12(

InchiKey: RFOHHLKIRBPFCX-UHFFFAOYSA-N

Formula: C18H15ClF2O5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 384.76

Physical Properties

Property code	Value	Unit	Source
gf	-687.41	kJ/mol	Joback Method
hf	-1017.45	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	86.33	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.308		Crippen Method
mcvol	253.490	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	895.49	K	Joback Method
tc	1115.21	K	Joback Method
tf	593.19	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.33	J/mol×K	895.49	Joback Method
cpg	738.05	J/mol×K	932.11	Joback Method
cpg	747.56	J/mol×K	968.73	Joback Method
cpg	755.84	J/mol×K	1005.35	Joback Method
cpg	762.89	J/mol×K	1041.97	Joback Method
cpg	768.72	J/mol×K	1078.59	Joback Method
cpg	773.33	J/mol×K	1115.21	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=U393448&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