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

Inchi: InChI=1S/C19H18ClFO4/c1-12-6-3-9-16(13(12)2)24-17(22)10-5-11-18(23)25-19-14(20)7

InchiKey: DKYISBXVIOBFTE-UHFFFAOYSA-N

Formula: C19H18ClFO4

SMILES: Cc1cccc(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)c1C

Mol. weight [g/mol]: 364.80

Physical Properties

Property code	Value	Unit	Source
gf	-379.18	kJ/mol	Joback Method
hf	-709.76	kJ/mol	Joback Method
hfus	44.34	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.777		Crippen Method
mcvol	259.940	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	896.68	K	Joback Method
tc	1121.49	K	Joback Method
tf	581.64	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.74	J/mol×K	896.68	Joback Method
cpg	762.68	J/mol×K	934.15	Joback Method
cpg	773.40	J/mol×K	971.62	Joback Method
cpg	782.92	J/mol×K	1009.09	Joback Method
cpg	791.27	J/mol×K	1046.56	Joback Method
cpg	798.45	J/mol×K	1084.03	Joback Method
cpg	804.48	J/mol×K	1121.49	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=U392224&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

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