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

Inchi: InChI=1S/C18H16ClFO4/c1-12-5-2-6-13(11-12)23-16(21)9-4-10-17(22)24-18-14(19)7-3-8

InchiKey: JLWIECBLDCHQSL-UHFFFAOYSA-N

Formula: C18H16ClFO4

SMILES: Cc1cccc(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)c1

Mol. weight [g/mol]: 350.77

Physical Properties

Property code	Value	Unit	Source
gf	-377.97	kJ/mol	Joback Method
hf	-677.65	kJ/mol	Joback Method
hfus	42.14	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.469		Crippen Method
mcvol	245.850	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	868.82	K	Joback Method
tc	1094.47	K	Joback Method
tf	557.85	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.81	J/mol×K	868.82	Joback Method
cpg	707.68	J/mol×K	906.43	Joback Method
cpg	718.38	J/mol×K	944.04	Joback Method
cpg	727.92	J/mol×K	981.65	Joback Method
cpg	736.34	J/mol×K	1019.26	Joback Method
cpg	743.66	J/mol×K	1056.87	Joback Method
cpg	749.88	J/mol×K	1094.47	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=U391959&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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