6-Fluoro-2-trifluoromethylbenzoic acid,4-chloro-2-methylphenyl ester

Other names: 6-Fluoro-2-trifluorobenzoic acid, 4-chloro-2-methylphenyl ester
Inchi: InChI=1S/C15H9ClF4O2/c1-8-7-9(16)5-6-12(8)22-14(21)13-10(15(18,19)20)3-2-4-11(13)
InchiKey: KWORTRPISKVFMR-UHFFFAOYSA-N
Formula: C15H9ClF4O2
SMILES: Cc1cc(Cl)ccc1OC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 332.68

Physical Properties

Property code	Value	Unit	Source
gf	-760.53	kJ/mol	Joback Method
hf	-979.48	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	65.16	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.026		Crippen Method
mcvol	201.450	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	723.45	K	Joback Method
tc	939.89	K	Joback Method
tf	468.59	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.63	J/mol×K	723.45	Joback Method
cpg	533.27	J/mol×K	759.52	Joback Method
cpg	544.00	J/mol×K	795.60	Joback Method
cpg	553.85	J/mol×K	831.67	Joback Method
cpg	562.87	J/mol×K	867.74	Joback Method
cpg	571.09	J/mol×K	903.82	Joback Method
cpg	578.58	J/mol×K	939.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343741&Units=SI
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

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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