6-Fluoro-2-trifluoromethylbenzoic acid, 3,4-dimethylphenyl ester

Other names: 6-Fluoro-2-trifluorobenzoic acid, 3,4-dimethylphenyl ester
Inchi: InChI=1S/C16H12F4O2/c1-9-6-7-11(8-10(9)2)22-15(21)14-12(16(18,19)20)4-3-5-13(14)1
InchiKey: FKXZGSHVIMZONQ-UHFFFAOYSA-N
Formula: C16H12F4O2
SMILES: Cc1ccc(OC(=O)c2c(F)cccc2C(F)(F)F)cc1C
Mol. weight [g/mol]: 312.26

Physical Properties

Property code	Value	Unit	Source
gf	-740.18	kJ/mol	Joback Method
hf	-984.38	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.681		Crippen Method
mcvol	203.300	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	708.90	K	Joback Method
tc	919.14	K	Joback Method
tf	449.94	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.34	J/mol×K	708.90	Joback Method
cpg	562.56	J/mol×K	743.94	Joback Method
cpg	574.83	J/mol×K	778.98	Joback Method
cpg	586.18	J/mol×K	814.02	Joback Method
cpg	596.66	J/mol×K	849.06	Joback Method
cpg	606.31	J/mol×K	884.10	Joback Method
cpg	615.18	J/mol×K	919.14	Joback Method

Sources

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=U343740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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