

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

Inchi:	InChI=1S/C16H12F4O2/c1-9-3-5-12(7-10(9)2)22-15(21)11-4-6-13(14(17)8-11)16(18,19)2
InchiKey:	KGMKSPLDVPCVCW-UHFFFAOYSA-N
Formula:	C16H12F4O2
SMILES:	Cc1ccc(OC(=O)c2ccc(C(F)(F)F)c(F)c2)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	1874.00		NIST Webbook
rinpol	1874.00		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/molxK	708.90	Joback Method
cpg	562.56	J/molxK	743.94	Joback Method
cpg	574.83	J/molxK	778.98	Joback Method
cpg	586.18	J/molxK	814.02	Joback Method
cpg	596.66	J/molxK	849.06	Joback Method
cpg	606.31	J/molxK	884.10	Joback Method
cpg	615.18	J/molxK	919.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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