

(3-Fluorophenyl) methanol, isopropyl ether

Inchi: InChI=1S/C10H13FO/c1-8(2)12-7-9-4-3-5-10(11)6-9/h3-6,8H,7H2,1-2H3
InchiKey: JAFQZVRJUASDQF-UHFFFAOYSA-N
Formula: C10H13FO
SMILES: CC(C)OCc1cccc(F)c1
Mol. weight [g/mol]: 168.21

Physical Properties

Property code	Value	Unit	Source
gf	-166.15	kJ/mol	Joback Method
hf	-358.28	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	42.00	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.751		Crippen Method
mcvol	135.640	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1124.00		NIST Webbook
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tb	481.11	K	Joback Method
tc	679.43	K	Joback Method
tf	249.22	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.11	J/molxK	481.11	Joback Method
cpg	304.07	J/molxK	514.16	Joback Method
cpg	317.37	J/molxK	547.22	Joback Method
cpg	330.03	J/molxK	580.27	Joback Method
cpg	342.05	J/molxK	613.33	Joback Method
cpg	353.45	J/molxK	646.38	Joback Method
cpg	364.23	J/molxK	679.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374626&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
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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