

(3-Fluorophenyl) methanol, tert.-butyl ether

Inchi:	InChI=1S/C11H15FO/c1-11(2,3)13-8-9-5-4-6-10(12)7-9/h4-7H,8H2,1-3H3
InchiKey:	YOKKPBRMFAVWTQ-UHFFFAOYSA-N
Formula:	C11H15FO
SMILES:	CC(C)(C)OCc1cccc(F)c1
Mol. weight [g/mol]:	182.23

Physical Properties

Property code	Value	Unit	Source
gf	-152.45	kJ/mol	Joback Method
hf	-382.39	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	43.31	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.141		Crippen Method
mcvol	149.730	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinsol	1191.00		NIST Webbook
tb	501.20	K	Joback Method
tc	704.94	K	Joback Method
tf	277.91	K	Joback Method
vc	0.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.29	J/mol×K	501.20	Joback Method
cpg	352.97	J/mol×K	535.16	Joback Method
cpg	367.75	J/mol×K	569.11	Joback Method
cpg	381.68	J/mol×K	603.07	Joback Method
cpg	394.79	J/mol×K	637.02	Joback Method
cpg	407.11	J/mol×K	670.98	Joback Method
cpg	418.67	J/mol×K	704.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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