

(3-Fluorophenyl) methanol, n-butyl ether

Inchi:	InChI=1S/C11H15FO/c1-2-3-7-13-9-10-5-4-6-11(12)8-10/h4-6,8H,2-3,7,9H2,1H3
InchiKey:	YPQRWVKXJWEPMG-UHFFFAOYSA-N
Formula:	C11H15FO
SMILES:	CCCCOCc1cccc(F)c1
Mol. weight [g/mol]:	182.23

Physical Properties

Property code	Value	Unit	Source
gf	-155.29	kJ/mol	Joback Method
hf	-373.64	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.142		Crippen Method
mcvol	149.730	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinsol	1264.00		NIST Webbook
tb	504.43	K	Joback Method
tc	696.06	K	Joback Method
tf	275.49	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.30	J/mol×K	504.43	Joback Method
cpg	348.82	J/mol×K	536.37	Joback Method
cpg	362.66	J/mol×K	568.31	Joback Method
cpg	375.84	J/mol×K	600.24	Joback Method
cpg	388.38	J/mol×K	632.18	Joback Method
cpg	400.29	J/mol×K	664.12	Joback Method
cpg	411.59	J/mol×K	696.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374628&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

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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