

(3-Fluorophenyl) methanol, n-propyl ether

Inchi:	InChI=1S/C10H13FO/c1-2-6-12-8-9-4-3-5-10(11)7-9/h3-5,7H,2,6,8H2,1H3
InchiKey:	QQFOJWSORNCKIS-UHFFFAOYSA-N
Formula:	C10H13FO
SMILES:	CCCOCC1CCCC(F)C1
Mol. weight [g/mol]:	168.21

Physical Properties

Property code	Value	Unit	Source
gf	-163.71	kJ/mol	Joback Method
hf	-353.00	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.752		Crippen Method
mcvol	135.640	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1165.00		NIST Webbook
tb	481.55	K	Joback Method
tc	675.51	K	Joback Method
tf	264.22	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.93	J/mol×K	481.55	Joback Method
cpg	303.51	J/mol×K	513.88	Joback Method
cpg	316.46	J/mol×K	546.20	Joback Method
cpg	328.80	J/mol×K	578.53	Joback Method
cpg	340.55	J/mol×K	610.86	Joback Method
cpg	351.70	J/mol×K	643.19	Joback Method
cpg	362.28	J/mol×K	675.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374627&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
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
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

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