(3-Fluorophenyl) methanol, 2-methylpropyl ether

Inchi: InChI=1S/C11H15FO/c1-9(2)7-13-8-10-4-3-5-11(12)6-10/h3-6,9H,7-8H2,1-2H3
InchiKey: INEUBKBRGSUFJV-UHFFFAOYSA-N
Formula: C11H15FO
SMILES: CC(C)COCc1cccc(F)c1
Mol. weight [g/mol]: 182.23

Physical Properties

Property code	Value	Unit	Source
gf	-157.73	kJ/mol	Joback Method
hf	-378.92	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.998		Crippen Method
mcvol	149.730	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1216.00		NIST Webbook
tb	503.99	K	Joback Method
tc	699.78	K	Joback Method
tf	260.49	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.52	J/mol×K	503.99	Joback Method
cpg	349.42	J/mol×K	536.62	Joback Method
cpg	363.62	J/mol×K	569.25	Joback Method
cpg	377.12	J/mol×K	601.89	Joback Method
cpg	389.93	J/mol×K	634.52	Joback Method
cpg	402.09	J/mol×K	667.15	Joback Method
cpg	413.58	J/mol×K	699.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374625&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
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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