(3-Fluorophenyl) methanol, 3-methylbutyl ether

Inchi: InChI=1S/C12H17FO/c1-10(2)6-7-14-9-11-4-3-5-12(13)8-11/h3-5,8,10H,6-7,9H2,1-2H3
InchiKey: PYLHVLPPIUYKDL-UHFFFAOYSA-N
Formula: C12H17FO
SMILES: CC(C)CCOCc1cccc(F)c1
Mol. weight [g/mol]: 196.26

Physical Properties

Property code	Value	Unit	Source
gf	-149.31	kJ/mol	Joback Method
hf	-399.56	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	46.45	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.388		Crippen Method
mcvol	163.820	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	526.87	K	Joback Method
tc	720.16	K	Joback Method
tf	271.76	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.83	J/mol×K	526.87	Joback Method
cpg	396.55	J/mol×K	559.09	Joback Method
cpg	411.52	J/mol×K	591.30	Joback Method
cpg	425.75	J/mol×K	623.52	Joback Method
cpg	439.26	J/mol×K	655.73	Joback Method
cpg	452.06	J/mol×K	687.95	Joback Method
cpg	464.18	J/mol×K	720.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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