(2-Fluorophenyl) methanol, n-pentyl ether

Inchi: InChI=1S/C12H17FO/c1-2-3-6-9-14-10-11-7-4-5-8-12(11)13/h4-5,7-8H,2-3,6,9-10H2,1H3
InchiKey: IYDQFFUMJKMMQH-UHFFFAOYSA-N
Formula: C12H17FO
SMILES: CCCCCOCc1ccccc1F
Mol. weight [g/mol]: 196.26

Physical Properties

Property code	Value	Unit	Source
gf	-146.87	kJ/mol	Joback Method
hf	-394.28	kJ/mol	Joback Method
hfus	24.76	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.533		Crippen Method
mcvol	163.820	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1360.00		NIST Webbook
tb	527.31	K	Joback Method
tc	716.64	K	Joback Method
tf	286.76	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.57	J/mol×K	527.31	Joback Method
cpg	395.91	J/mol×K	558.86	Joback Method
cpg	410.52	J/mol×K	590.42	Joback Method
cpg	424.44	J/mol×K	621.97	Joback Method
cpg	437.68	J/mol×K	653.53	Joback Method
cpg	450.24	J/mol×K	685.08	Joback Method
cpg	462.15	J/mol×K	716.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374569&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