(4-Fluorophenyl) methanol, neopentyl ether

Inchi: InChI=1S/C12H17FO/c1-12(2,3)9-14-8-10-4-6-11(13)7-5-10/h4-7H,8-9H2,1-3H3
InchiKey: IODTUJJPFDTQAM-UHFFFAOYSA-N
Formula: C12H17FO
SMILES: CC(C)(C)COCc1ccc(F)cc1
Mol. weight [g/mol]: 196.26

Physical Properties

Property code	Value	Unit	Source
gf	-144.03	kJ/mol	Joback Method
hf	-403.03	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	45.54	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.388		Crippen Method
mcvol	163.820	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1240.00		NIST Webbook
tb	524.08	K	Joback Method
tc	724.94	K	Joback Method
tf	289.18	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.60	J/mol×K	524.08	Joback Method
cpg	400.03	J/mol×K	557.56	Joback Method
cpg	415.54	J/mol×K	591.03	Joback Method
cpg	430.16	J/mol×K	624.51	Joback Method
cpg	443.92	J/mol×K	657.99	Joback Method
cpg	456.87	J/mol×K	691.47	Joback Method
cpg	469.04	J/mol×K	724.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374643&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