2-Bromo-5-fluorobenzyl alcohol, n-pentyl ether

Inchi: InChI=1S/C12H16BrFO/c1-2-3-4-7-15-9-10-8-11(14)5-6-12(10)13/h5-6,8H,2-4,7,9H2,1H3
InchiKey: HLTOJTJXMOLFPS-UHFFFAOYSA-N
Formula: C12H16BrFO
SMILES: CCCCCOCc1cc(F)ccc1Br
Mol. weight [g/mol]: 275.16

Physical Properties

Property code	Value	Unit	Source
gf	-142.18	kJ/mol	Joback Method
hf	-379.42	kJ/mol	Joback Method
hfus	29.65	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.295		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	598.45	K	Joback Method
tc	801.70	K	Joback Method
tf	359.08	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.29	J/mol×K	598.45	Joback Method
cpg	438.46	J/mol×K	632.33	Joback Method
cpg	451.89	J/mol×K	666.20	Joback Method
cpg	464.58	J/mol×K	700.08	Joback Method
cpg	476.56	J/mol×K	733.95	Joback Method
cpg	487.86	J/mol×K	767.83	Joback Method
cpg	498.49	J/mol×K	801.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375221&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