2-Bromo-5-fluorobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H14BrFO/c1-8(2)6-14-7-9-5-10(13)3-4-11(9)12/h3-5,8H,6-7H2,1-2H3
InchiKey: ROPJBLWBIZZMJV-UHFFFAOYSA-N
Formula: C11H14BrFO
SMILES: CC(C)COCc1cc(F)ccc1Br
Mol. weight [g/mol]: 261.13

Physical Properties

Property code	Value	Unit	Source
gf	-153.04	kJ/mol	Joback Method
hf	-364.06	kJ/mol	Joback Method
hfus	23.54	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.761		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	575.13	K	Joback Method
tc	785.81	K	Joback Method
tf	332.81	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.65	J/mol×K	575.13	Joback Method
cpg	390.42	J/mol×K	610.24	Joback Method
cpg	403.45	J/mol×K	645.36	Joback Method
cpg	415.73	J/mol×K	680.47	Joback Method
cpg	427.31	J/mol×K	715.58	Joback Method
cpg	438.20	J/mol×K	750.70	Joback Method
cpg	448.41	J/mol×K	785.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375230&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