2-Bromo-5-fluorobenzyl alcohol, tert.-butyl ether

Inchi: InChI=1S/C11H14BrFO/c1-11(2,3)14-7-8-6-9(13)4-5-10(8)12/h4-6H,7H2,1-3H3
InchiKey: YGLXCCJAAKQZSM-UHFFFAOYSA-N
Formula: C11H14BrFO
SMILES: CC(C)(C)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 261.13

Physical Properties

Property code	Value	Unit	Source
gf	-147.76	kJ/mol	Joback Method
hf	-367.53	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.903		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
tb	572.34	K	Joback Method
tc	791.36	K	Joback Method
tf	350.23	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.71	J/mol×K	572.34	Joback Method
cpg	393.95	J/mol×K	608.84	Joback Method
cpg	407.28	J/mol×K	645.35	Joback Method
cpg	419.74	J/mol×K	681.85	Joback Method
cpg	431.38	J/mol×K	718.36	Joback Method
cpg	442.24	J/mol×K	754.86	Joback Method
cpg	452.37	J/mol×K	791.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375222&Units=SI

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