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

Inchi: InChI=1S/C12H16BrFO/c1-3-9(2)7-15-8-10-6-11(14)4-5-12(10)13/h4-6,9H,3,7-8H2,1-2H
InchiKey: KYUQIOAWSMKHJX-UHFFFAOYSA-N
Formula: C12H16BrFO
SMILES: CCC(C)COCc1cc(F)ccc1Br
Mol. weight [g/mol]: 275.16

Physical Properties

Property code	Value	Unit	Source
gf	-144.62	kJ/mol	Joback Method
hf	-384.70	kJ/mol	Joback Method
hfus	26.13	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.151		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1563.00		NIST Webbook
tb	598.01	K	Joback Method
tc	805.35	K	Joback Method
tf	344.08	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.70	J/mol×K	598.01	Joback Method
cpg	439.22	J/mol×K	632.57	Joback Method
cpg	452.94	J/mol×K	667.12	Joback Method
cpg	465.89	J/mol×K	701.68	Joback Method
cpg	478.09	J/mol×K	736.23	Joback Method
cpg	489.57	J/mol×K	770.79	Joback Method
cpg	500.34	J/mol×K	805.35	Joback Method

Sources

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=U375224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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