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

Inchi: InChI=1S/C11H14BrFO/c1-2-3-6-14-8-9-7-10(13)4-5-11(9)12/h4-5,7H,2-3,6,8H2,1H3
InchiKey: DHULEFKNXCFIAJ-UHFFFAOYSA-N
Formula: C11H14BrFO
SMILES: CCCCOCc1cc(F)ccc1Br
Mol. weight [g/mol]: 261.13

Physical Properties

Property code	Value	Unit	Source
gf	-150.60	kJ/mol	Joback Method
hf	-358.78	kJ/mol	Joback Method
hfus	27.06	kJ/mol	Joback Method
hvap	51.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.905		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	575.57	K	Joback Method
tc	781.93	K	Joback Method
tf	347.81	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.26	J/mol×K	575.57	Joback Method
cpg	389.69	J/mol×K	609.96	Joback Method
cpg	402.41	J/mol×K	644.36	Joback Method
cpg	414.44	J/mol×K	678.75	Joback Method
cpg	425.80	J/mol×K	713.14	Joback Method
cpg	436.50	J/mol×K	747.53	Joback Method
cpg	446.56	J/mol×K	781.93	Joback Method

Sources

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=U375226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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