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

Inchi: InChI=1S/C10H12BrFO/c1-2-5-13-7-8-6-9(12)3-4-10(8)11/h3-4,6H,2,5,7H2,1H3

InchiKey: ADTQNBLCGVLSJB-UHFFFAOYSA-N

Formula: C10H12BrFO

SMILES: CCCOCc1cc(F)ccc1Br

Mol. weight [g/mol]: 247.10

Physical Properties

Property code	Value	Unit	Source
gf	-159.02	kJ/mol	Joback Method
hf	-338.14	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	49.48	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.515		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1407.00		NIST Webbook
tb	552.69	K	Joback Method
tc	762.33	K	Joback Method
tf	336.54	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.92	J/mol×K	552.69	Joback Method
cpg	342.50	J/mol×K	587.63	Joback Method
cpg	354.42	J/mol×K	622.57	Joback Method
cpg	365.68	J/mol×K	657.51	Joback Method
cpg	376.31	J/mol×K	692.45	Joback Method
cpg	386.32	J/mol×K	727.39	Joback Method
cpg	395.73	J/mol×K	762.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375227&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

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