2-Bromo-5-fluorobenzyl alcohol, isopropyl ether

Inchi: InChI=1S/C10H12BrFO/c1-7(2)13-6-8-5-9(12)3-4-10(8)11/h3-5,7H,6H2,1-2H3
InchiKey: YIAWMCYBOIIBIQ-UHFFFAOYSA-N
Formula: C10H12BrFO
SMILES: CC(C)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 247.10

Physical Properties

Property code	Value	Unit	Source
gf	-161.46	kJ/mol	Joback Method
hf	-343.42	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.513		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook
tb	552.25	K	Joback Method
tc	766.46	K	Joback Method
tf	321.54	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.29	J/mol×K	552.25	Joback Method
cpg	343.21	J/mol×K	587.95	Joback Method
cpg	355.42	J/mol×K	623.65	Joback Method
cpg	366.94	J/mol×K	659.36	Joback Method
cpg	377.79	J/mol×K	695.06	Joback Method
cpg	387.99	J/mol×K	730.76	Joback Method
cpg	397.56	J/mol×K	766.46	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=U375228&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

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