4-Bromo-2,6-difluorobenzyl alcohol, ethyl ether

Inchi: InChI=1S/C9H9BrF2O/c1-2-13-5-7-8(11)3-6(10)4-9(7)12/h3-4H,2,5H2,1H3
InchiKey: BSJBEBZSGQTJQN-UHFFFAOYSA-N
Formula: C9H9BrF2O
SMILES: CCOCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 251.07

Physical Properties

Property code	Value	Unit	Source
gf	-371.88	kJ/mol	Joback Method
hf	-525.08	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.264		Crippen Method
mcvol	140.820	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
tb	534.06	K	Joback Method
tc	737.69	K	Joback Method
tf	338.38	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.23	J/mol×K	534.06	Joback Method
cpg	303.94	J/mol×K	568.00	Joback Method
cpg	314.12	J/mol×K	601.94	Joback Method
cpg	323.79	J/mol×K	635.87	Joback Method
cpg	332.96	J/mol×K	669.81	Joback Method
cpg	341.63	J/mol×K	703.75	Joback Method
cpg	349.82	J/mol×K	737.69	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=U375291&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