4-Bromo-2,6-difluorobenzyl alcohol, n-propyl ether

Inchi: InChI=1S/C10H11BrF2O/c1-2-3-14-6-8-9(12)4-7(11)5-10(8)13/h4-5H,2-3,6H2,1H3
InchiKey: VXROEDKIUVVMKW-UHFFFAOYSA-N
Formula: C10H11BrF2O
SMILES: CCCOCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 265.10

Physical Properties

Property code	Value	Unit	Source
gf	-363.46	kJ/mol	Joback Method
hf	-545.72	kJ/mol	Joback Method
hfus	27.16	kJ/mol	Joback Method
hvap	49.33	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.654		Crippen Method
mcvol	154.910	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1366.00		NIST Webbook
tb	556.94	K	Joback Method
tc	757.61	K	Joback Method
tf	349.65	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.69	J/mol×K	556.94	Joback Method
cpg	349.37	J/mol×K	590.39	Joback Method
cpg	360.49	J/mol×K	623.83	Joback Method
cpg	371.04	J/mol×K	657.28	Joback Method
cpg	381.04	J/mol×K	690.72	Joback Method
cpg	390.49	J/mol×K	724.17	Joback Method
cpg	399.42	J/mol×K	757.61	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=U375287&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