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

Inchi: InChI=1S/C10H11BrF2O/c1-6(2)14-5-8-9(12)3-7(11)4-10(8)13/h3-4,6H,5H2,1-2H3
InchiKey: NWZOZCZPIHKOKH-UHFFFAOYSA-N
Formula: C10H11BrF2O
SMILES: CC(C)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 265.10

Physical Properties

Property code	Value	Unit	Source
gf	-365.90	kJ/mol	Joback Method
hf	-551.00	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.652		Crippen Method
mcvol	154.910	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
tb	556.50	K	Joback Method
tc	761.39	K	Joback Method
tf	334.65	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.07	J/mol×K	556.50	Joback Method
cpg	350.06	J/mol×K	590.65	Joback Method
cpg	361.45	J/mol×K	624.80	Joback Method
cpg	372.24	J/mol×K	658.95	Joback Method
cpg	382.44	J/mol×K	693.09	Joback Method
cpg	392.07	J/mol×K	727.24	Joback Method
cpg	401.15	J/mol×K	761.39	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=U375289&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