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

Inchi: InChI=1S/C11H13BrF2O/c1-2-3-4-15-7-9-10(13)5-8(12)6-11(9)14/h5-6H,2-4,7H2,1H3
InchiKey: YUDUSRDVJBNDJT-UHFFFAOYSA-N
Formula: C11H13BrF2O
SMILES: CCCCOCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 279.12

Physical Properties

Property code	Value	Unit	Source
gf	-355.04	kJ/mol	Joback Method
hf	-566.36	kJ/mol	Joback Method
hfus	29.75	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.044		Crippen Method
mcvol	169.000	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	579.82	K	Joback Method
tc	777.69	K	Joback Method
tf	360.92	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.95	J/mol×K	579.82	Joback Method
cpg	396.50	J/mol×K	612.80	Joback Method
cpg	408.43	J/mol×K	645.78	Joback Method
cpg	419.75	J/mol×K	678.75	Joback Method
cpg	430.48	J/mol×K	711.73	Joback Method
cpg	440.62	J/mol×K	744.71	Joback Method
cpg	450.20	J/mol×K	777.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375286&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