2-Bromo-5-fluorobenzyl alcohol, neopentyl ether

Inchi: InChI=1S/C12H16BrFO/c1-12(2,3)8-15-7-9-6-10(14)4-5-11(9)13/h4-6H,7-8H2,1-3H3
InchiKey: DRTHHCVALBSBOM-UHFFFAOYSA-N
Formula: C12H16BrFO
SMILES: CC(C)(C)COCc1cc(F)ccc1Br
Mol. weight [g/mol]: 275.16

Physical Properties

Property code	Value	Unit	Source
gf	-139.34	kJ/mol	Joback Method
hf	-388.17	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.151		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1481.00		NIST Webbook
tb	595.22	K	Joback Method
tc	810.44	K	Joback Method
tf	361.50	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.62	J/mol×K	595.22	Joback Method
cpg	442.55	J/mol×K	631.09	Joback Method
cpg	456.55	J/mol×K	666.96	Joback Method
cpg	469.65	J/mol×K	702.83	Joback Method
cpg	481.91	J/mol×K	738.70	Joback Method
cpg	493.37	J/mol×K	774.57	Joback Method
cpg	504.07	J/mol×K	810.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375220&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

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