2,3,4,5,6-Pentabromobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H11Br5O/c1-5(2)3-17-4-6-7(12)9(14)11(16)10(15)8(6)13/h5H,3-4H2,1-2H3

InchiKey: AZZMIYVXZOUIHE-UHFFFAOYSA-N

Formula: C11H11Br5O

SMILES: CC(C)COCc1c(Br)c(Br)c(Br)c(Br)c1Br

Mol. weight [g/mol]: 558.72

Physical Properties

Property code	Value	Unit	Source
gf	70.16	kJ/mol	Joback Method
hf	-97.04	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	6.672		Crippen Method
mcvol	235.460	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	855.44	K	Joback Method
tc	1120.50	K	Joback Method
tf	608.98	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.55	J/mol×K	855.44	Joback Method
cpg	498.73	J/mol×K	899.62	Joback Method
cpg	507.32	J/mol×K	943.79	Joback Method
cpg	515.38	J/mol×K	987.97	Joback Method
cpg	522.98	J/mol×K	1032.15	Joback Method
cpg	530.20	J/mol×K	1076.32	Joback Method
cpg	537.10	J/mol×K	1120.50	Joback Method
dvisc	0.0002791	Pa×s	608.98	Joback Method

dvisc	0.0002107	Pa×s	650.06	Joback Method
dvisc	0.0001645	Pa×s	691.13	Joback Method
dvisc	0.0001321	Pa×s	732.21	Joback Method
dvisc	0.0001085	Pa×s	773.29	Joback Method
dvisc	0.0000910	Pa×s	814.36	Joback Method
dvisc	0.0000775	Pa×s	855.44	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=U375317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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