2,3,4,5,6-Pentabromobenzyl alcohol, n-propyl ether

Inchi: InChI=1S/C10H9Br5O/c1-2-3-16-4-5-6(11)8(13)10(15)9(14)7(5)12/h2-4H2,1H3
InchiKey: BUKHQPTWTSHKBX-UHFFFAOYSA-N
Formula: C10H9Br5O
SMILES: CCCOCc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]: 544.70

Physical Properties

Property code	Value	Unit	Source
gf	64.18	kJ/mol	Joback Method
hf	-71.12	kJ/mol	Joback Method
hfus	41.37	kJ/mol	Joback Method
hvap	78.02	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	6.426		Crippen Method
mcvol	221.370	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	2621.00		NIST Webbook
tb	833.00	K	Joback Method
tc	1099.01	K	Joback Method
tf	612.71	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.54	J/mol×K	833.00	Joback Method
cpg	444.87	J/mol×K	877.34	Joback Method
cpg	452.67	J/mol×K	921.67	Joback Method
cpg	460.01	J/mol×K	966.01	Joback Method
cpg	466.95	J/mol×K	1010.34	Joback Method
cpg	473.56	J/mol×K	1054.68	Joback Method
cpg	479.89	J/mol×K	1099.01	Joback Method
dvisc	0.0002979	Pa×s	612.71	Joback Method
dvisc	0.0002349	Pa×s	649.43	Joback Method

dvisc	0.0001900	Pa×s	686.14	Joback Method
dvisc	0.0001570	Pa×s	722.86	Joback Method
dvisc	0.0001322	Pa×s	759.57	Joback Method
dvisc	0.0001130	Pa×s	796.29	Joback Method
dvisc	0.0000980	Pa×s	833.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375315&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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