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

Inchi: InChI=1S/C9H7Br5O/c1-2-15-3-4-5(10)7(12)9(14)8(13)6(4)11/h2-3H2,1H3
InchiKey: XFODZBFAUIPPPP-UHFFFAOYSA-N
Formula: C9H7Br5O
SMILES: CCOCc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]: 530.67

Physical Properties

Property code	Value	Unit	Source
gf	55.76	kJ/mol	Joback Method
hf	-50.48	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	75.80	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.036		Crippen Method
mcvol	207.280	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
rinpol	2534.00		NIST Webbook
tb	810.12	K	Joback Method
tc	1082.43	K	Joback Method
tf	601.44	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.33	J/mol×K	810.12	Joback Method
cpg	418.59	J/mol×K	1037.05	Joback Method
cpg	412.66	J/mol×K	991.66	Joback Method
cpg	406.44	J/mol×K	946.28	Joback Method
cpg	399.85	J/mol×K	900.89	Joback Method
cpg	392.84	J/mol×K	855.51	Joback Method
cpg	424.28	J/mol×K	1082.43	Joback Method
dvisc	0.0001132	Pa×s	810.12	Joback Method
dvisc	0.0001299	Pa×s	775.34	Joback Method

dvisc	0.0001509	Pa×s	740.56	Joback Method
dvisc	0.0001780	Pa×s	705.78	Joback Method
dvisc	0.0002136	Pa×s	671.00	Joback Method
dvisc	0.0002614	Pa×s	636.22	Joback Method
dvisc	0.0003276	Pa×s	601.44	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=U375318&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
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