2,3,5-Triiodobenzyl alcohol

Inchi: InChI=1S/C7H5I3O/c8-5-1-4(3-11)7(10)6(9)2-5/h1-2,11H,3H2
InchiKey: KFZNKUWVRXKLJP-UHFFFAOYSA-N
Formula: C7H5I3O
SMILES: OCc1cc(I)cc(I)c1I
Mol. weight [g/mol]: 485.83
CAS: 31075-53-3

Physical Properties

Property code	Value	Unit	Source
gf	129.12	kJ/mol	Joback Method
hf	92.69	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	2.993		Crippen Method
mcvol	169.060	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	2402.00		NIST Webbook
tb	772.78	K	Joback Method
tc	1059.35	K	Joback Method
tf	467.63	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.11	J/mol×K	772.78	Joback Method
cpg	280.70	J/mol×K	820.54	Joback Method
cpg	285.90	J/mol×K	868.30	Joback Method
cpg	290.80	J/mol×K	916.06	Joback Method
cpg	295.51	J/mol×K	963.83	Joback Method
cpg	300.12	J/mol×K	1011.59	Joback Method
cpg	304.73	J/mol×K	1059.35	Joback Method
dvisc	0.0009811	Pa×s	467.63	Joback Method

dvisc	0.0004577	Pa×s	518.49	Joback Method
dvisc	0.0002447	Pa×s	569.35	Joback Method
dvisc	0.0001450	Pa×s	620.20	Joback Method
dvisc	0.0000930	Pa×s	671.06	Joback Method
dvisc	0.0000635	Pa×s	721.92	Joback Method
dvisc	0.0000456	Pa×s	772.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31075533&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