2,3,5-Triiodobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H13I3O/c1-2-3-4-15-7-8-5-9(12)6-10(13)11(8)14/h5-6H,2-4,7H2,1H3
InchiKey: YZCUYJDABIDFNK-UHFFFAOYSA-N
Formula: C11H13I3O
SMILES: CCCCOCc1cc(I)cc(I)c1I
Mol. weight [g/mol]: 541.93

Physical Properties

Property code	Value	Unit	Source
gf	194.62	kJ/mol	Joback Method
hf	30.14	kJ/mol	Joback Method
hfus	31.53	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	4.817		Crippen Method
mcvol	225.420	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	2508.00		NIST Webbook
rinpol	2508.00		NIST Webbook
tb	794.54	K	Joback Method
tc	1077.66	K	Joback Method
tf	474.12	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.37	J/mol×K	794.54	Joback Method
cpg	473.56	J/mol×K	841.73	Joback Method
cpg	483.87	J/mol×K	888.91	Joback Method
cpg	493.40	J/mol×K	936.10	Joback Method
cpg	502.22	J/mol×K	983.29	Joback Method
cpg	510.43	J/mol×K	1030.47	Joback Method
cpg	518.11	J/mol×K	1077.66	Joback Method
dvisc	0.0007897	Pa×s	474.12	Joback Method

dvisc	0.0004716	Pa×s	527.52	Joback Method
dvisc	0.0003096	Pa×s	580.93	Joback Method
dvisc	0.0002182	Pa×s	634.33	Joback Method
dvisc	0.0001624	Pa×s	687.73	Joback Method
dvisc	0.0001261	Pa×s	741.14	Joback Method
dvisc	0.0001013	Pa×s	794.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375219&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