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

Inchi: InChI=1S/C12H15I3O/c1-2-3-4-5-16-8-9-6-10(13)7-11(14)12(9)15/h6-7H,2-5,8H2,1H3
InchiKey: NCVFDQAOZDYPAS-UHFFFAOYSA-N
Formula: C12H15I3O
SMILES: CCCCCOCc1cc(I)cc(I)c1I
Mol. weight [g/mol]: 555.96

Physical Properties

Property code	Value	Unit	Source
gf	203.04	kJ/mol	Joback Method
hf	9.50	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.207		Crippen Method
mcvol	239.510	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	2615.00		NIST Webbook
tb	817.42	K	Joback Method
tc	1093.41	K	Joback Method
tf	485.39	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	817.42	Joback Method
cpg	565.83	J/mol×K	1047.42	Joback Method
cpg	557.06	J/mol×K	1001.42	Joback Method
cpg	547.67	J/mol×K	955.42	Joback Method
cpg	537.55	J/mol×K	909.42	Joback Method
cpg	526.62	J/mol×K	863.42	Joback Method
cpg	574.05	J/mol×K	1093.41	Joback Method
dvisc	0.0000878	Pa×s	817.42	Joback Method
dvisc	0.0001097	Pa×s	762.08	Joback Method

dvisc	0.0001419	Pa×s	706.74	Joback Method
dvisc	0.0001919	Pa×s	651.40	Joback Method
dvisc	0.0002743	Pa×s	596.07	Joback Method
dvisc	0.0004220	Pa×s	540.73	Joback Method
dvisc	0.0007162	Pa×s	485.39	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=U375232&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