

2,3,5-Triiodobenzyl alcohol, isopropyl ether

Inchi:	InChI=1S/C10H11I3O/c1-6(2)14-5-7-3-8(11)4-9(12)10(7)13/h3-4,6H,5H2,1-2H3
InchiKey:	OQEDESKZDRQXPB-UHFFFAOYSA-N
Formula:	C10H11I3O
SMILES:	CC(C)OCc1cc(I)cc(I)c1I
Mol. weight [g/mol]:	527.91

Physical Properties

Property code	Value	Unit	Source
gf	183.76	kJ/mol	Joback Method
hf	45.50	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.425		Crippen Method
mvol	211.330	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	2335.00		NIST Webbook
tb	771.22	K	Joback Method
tc	1068.44	K	Joback Method
tf	447.85	K	Joback Method
vc	0.763	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.78	J/molxK	771.22	Joback Method
cpg	422.45	J/molxK	820.76	Joback Method
cpg	432.21	J/molxK	870.29	Joback Method
cpg	441.15	J/molxK	919.83	Joback Method
cpg	449.38	J/molxK	969.37	Joback Method
cpg	456.97	J/molxK	1018.90	Joback Method
cpg	464.02	J/molxK	1068.44	Joback Method
dvisc	0.0009758	Paxs	447.85	Joback Method
dvisc	0.0005543	Paxs	501.75	Joback Method

dvisc	0.0003514	Paxs	555.64	Joback Method
dvisc	0.0002415	Paxs	609.53	Joback Method
dvisc	0.0001763	Paxs	663.43	Joback Method
dvisc	0.0001350	Paxs	717.32	Joback Method
dvisc	0.0001073	Paxs	771.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375238&Units=SI

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

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