

3,5-Diiodo-2-hydroxybenzaldehyde

Other names:	Benzaldehyde, 2-hydroxy-3,5-diiodo-
Inchi:	InChI=1S/C7H4I2O2/c8-5-1-4(3-10)7(11)6(9)2-5/h1-3,11H
InchiKey:	MYWSBJKVOUZCIA-UHFFFAOYSA-N
Formula:	C7H4I2O2
SMILES:	O=Cc1cc(I)cc(I)c1O
Mol. weight [g/mol]:	373.91

Physical Properties

Property code	Value	Unit	Source
hfus	24.03	kJ/mol	Joback Method
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.414		Crippen Method
mcvol	144.810	ml/mol	McGowan Method
tf	414.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.36	J/mol×K	711.76	Joback Method
cpg	261.18	J/mol×K	761.24	Joback Method
cpg	266.62	J/mol×K	810.73	Joback Method
cpg	271.89	J/mol×K	860.21	Joback Method
cpg	277.15	J/mol×K	909.69	Joback Method
cpg	282.62	J/mol×K	959.17	Joback Method
cpg	288.46	J/mol×K	1008.66	Joback Method
dvisc	0.0004535	Pa×s	489.95	Joback Method
dvisc	0.0002444	Pa×s	526.92	Joback Method
dvisc	0.0001429	Pa×s	563.89	Joback Method
dvisc	0.0000892	Pa×s	600.86	Joback Method
dvisc	0.0000588	Pa×s	637.82	Joback Method
dvisc	0.0000406	Pa×s	674.79	Joback Method
dvisc	0.0000291	Pa×s	711.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631778&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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