

2-Hydroxyiminodibenzyl

Inchi:	InChI=1S/C14H13NO/c16-12-7-8-14-11(9-12)6-5-10-3-1-2-4-13(10)15-14/h1-4,7-9,15-16
InchiKey:	DWEDVKMRFXQLQH-UHFFFAOYSA-N
Formula:	C14H13NO
SMILES:	Oc1ccc2c(c1)CCc1ccccc1N2
Mol. weight [g/mol]:	211.26

Physical Properties

Property code	Value	Unit	Source
gf	274.11	kJ/mol	Joback Method
hf	71.47	kJ/mol	Joback Method
hfus	31.76	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.234		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpola	2265.00		NIST Webbook
rinpola	2265.00		NIST Webbook
tb	723.62	K	Joback Method
tc	992.85	K	Joback Method
tf	564.35	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.18	J/mol×K	723.62	Joback Method
cpg	462.55	J/mol×K	768.49	Joback Method
cpg	475.91	J/mol×K	813.36	Joback Method
cpg	488.46	J/mol×K	858.23	Joback Method
cpg	500.42	J/mol×K	903.10	Joback Method
cpg	511.99	J/mol×K	947.97	Joback Method
cpg	523.38	J/mol×K	992.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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