

1,2-CYCLOHEXANEDIONE DIOXIME

Other names:	Nioxime 1,2-Cyclohexadione dioxime Nioxim 1,2-Bis(hydroxyimino)cyclohexane Cyclohexan-1,2-dion-dioxim Cyclohexan-1,2-dion-dioxime cyclohexane-1,2-dione dioxime
Inchi:	InChI=1S/C6H10N2O2/c9-7-5-3-1-2-4-6(5)8-10/h9-10H,1-4H2
InchiKey:	CUNNCKOPAWXYDX-UHFFFAOYSA-N
Formula:	C6H10N2O2
SMILES:	ON=C1CCCCC1=NO
Mol. weight [g/mol]:	142.16

Physical Properties

Property code	Value	Unit	Source
chs	-3657.60	kJ/mol	NIST Webbook
hf	-69.66	kJ/mol	NIST Webbook
hsub	62.00 ± 17.00	kJ/mol	NIST Webbook
hvap	87.97	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
logp	1.221		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
tb	537.71	K	Cheméo Relay (1.0)
tf	387.05	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C492999&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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