

Phthalazin-1-one

Other names:	1(2H)-phthalazinone 1-Phthalazinol Phthalazinone Phthalazone phthalazin-1(2H)-one
Inchi:	InChI=1S/C8H6N2O/c11-8-7-4-2-1-3-6(7)5-9-10-8/h1-5H,(H,10,11)
InchiKey:	IJAPPYDYQCXOEF-UHFFFAOYSA-N
Formula:	C8H6N2O
SMILES:	Oc1nncc2ccccc12
Mol. weight [g/mol]:	146.15
CAS:	119-39-1

Physical Properties

Property code	Value	Unit	Source
hsub	107.40 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	1.335		Crippen Method
mvol	106.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	104.40 ± 0.50	kJ/mol	358.00	NIST Webbook
rhos	1290.00	kg/m ³	298.15	Experimental study on the thermochemistry of 1-(2H)-phthalazinone and phthalhydrazide

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C119391&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Experimental study on the thermochemistry of 1-(2H)-phthalazinone and phthalhydrazide: <https://www.doi.org/10.1016/j.jct.2008.01.010>

Legend

hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rhos: Solid Density

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