1,4-DIOXO-1,2,3,4-TETRAHYDROPHTHALAZINE

Other names:	Phthalhydrazide
	1,4-Phthalazinedione, 2,3-dihydro-
	Phthalazine-1,4-dione
	Phthalazine-1,4(2H,3H)-dione
	2,3-dihydrophthalazine-1,4-dione
Inchi:	InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)8(12)10-9-7/h1-4H,(H,9,11)(H,10,12)
InchiKey:	KGLPWQKSKUVKMJ-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	O=c1[nH][nH]c(=O)c2ccccc12
Mol. weight [g/mol]:	162.15

Physical Properties

Property code	Value	Unit	Source
hf	-123.54	kJ/mol	Cheméo Relay (1.0)
hsub	139.80 ± 0.70	kJ/mol	NIST Webbook
hvap	113.97	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-1.58		Cheméo Relay (1.0)
logp	-0.747		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	5139.54	kPa	Cheméo Relay (1.0, beta)
tb	607.72	K	Cheméo Relay (1.0)
tc	910.08	K	Cheméo Relay (1.0)
tf	521.07	K	Cheméo Relay (1.0)
vc	0.403	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	132.70 ± 0.70	kJ/mol	439.00	NIST Webbook

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=C1445698&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume