quinazoline-2,4(1H,3H)-dione

Other names:	2,4(1H,3H)-quinazolinedione
	benzoyleneurea
Inchi:	InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)9-8(12)10-7/h1-4H,(H2,9,10,11,12)
InchiKey:	SDQJTWBNWQABLE-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	O=c1[nH]c(=O)c2ccccc2[nH]1
Mol. weight [g/mol]:	162.15

Physical Properties

Property code	Value	Unit	Source
hf	-193.40	kJ/mol	Cheméo Relay (1.0)
hfus	128.30	kJ/mol	Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-2.04		Cheméo Relay (1.0)
logp	-0.747		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	5466.24	kPa	Cheméo Relay (1.0, beta)
tb	622.10	K	Cheméo Relay (1.0)
tc	920.84	K	Cheméo Relay (1.0)
tf	545.99	K	Cheméo Relay (1.0)
vc	0.404	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study:	https://www.doi.org/10.1021/je2004929
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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