BENZO[A]PHENAZINE

Inchi: InChI=1S/C16H10N2/c1-2-6-12-11(5-1)9-10-15-16(12)18-14-8-4-3-7-13(14)17-15/h1-10H
InchiKey: SEXRCKWGFSXUOO-UHFFFAOYSA-N
Formula: C16H10N2
SMILES: c1ccc2c(c1)ccc1nc3ccccc3nc12
Mol. weight [g/mol]: 230.27

Physical Properties

Property code	Value	Unit	Source
hf	378.09	kJ/mol	Cheméo Relay (1.0)
hvap	107.13	kJ/mol	Cheméo Relay (1.0)
ie	7.88	eV	Cheméo Relay (1.0)
log10ws	-4.99		Cheméo Relay (1.0)
logp	3.936		Crippen Method
mcvol	174.120	ml/mol	McGowan Method
pc	3766.18	kPa	Cheméo Relay (1.0, beta)
tb	688.31	K	Cheméo Relay (1.0)
tc	1028.15	K	Cheméo Relay (1.0)
tf	443.02	K	Cheméo Relay (1.0)
vc	0.677	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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C225616&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
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