

Benzo[c]cinnoline

Other names:	9,10-Diazaphenanthrene Diphenylenazone Phenazone Phenazone (three-ring system) 2,2'-Azobiphenyl 3,4-Benzocinnoline 5,6-Phenanthroline o-Diphenyleneazine 5,6-Diazaphenanthrene NSC 86935
Inchi:	InChI=1S/C12H8N2/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)14-13-11/h1-8H
InchiKey:	SWJXWSAKHXBQSY-UHFFFAOYSA-N
Formula:	C12H8N2
SMILES:	<chem>c1ccc2c(c1)nnc1cccc12</chem>
Mol. weight [g/mol]:	180.21
CAS:	230-17-1

Physical Properties

Property code	Value	Unit	Source
chs	-6160.50 ± 1.70	kJ/mol	NIST Webbook
chs	-6144.80 ± 3.80	kJ/mol	NIST Webbook
ea	0.92 ± 0.10	eV	NIST Webbook
hf	391.70	kJ/mol	NIST Webbook
hf	376.00 ± 4.90	kJ/mol	NIST Webbook
hfs	295.10	kJ/mol	NIST Webbook
hfs	279.40 ± 4.00	kJ/mol	NIST Webbook
hsub	96.60	kJ/mol	NIST Webbook
hsub	96.55 ± 0.90	kJ/mol	NIST Webbook
hsub	101.68 ± 0.18	kJ/mol	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	8.69 ± 0.02	eV	NIST Webbook
log10ws	-4.61		Crippen Method
logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
rinpol	1933.00		NIST Webbook
rinpol	322.07		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.90	kJ/mol	429.00	NIST Webbook
hfust	20.92	kJ/mol	432.20	NIST Webbook
hfust	20.92	kJ/mol	432.20	NIST Webbook
hsubt	101.70 ± 0.20	kJ/mol	340.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C230171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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