DIBENZ[A,C]ACRIDINE

Inchi: InChI=1S/C21H13N/c1-6-12-20-14(7-1)13-19-17-10-3-2-8-15(17)16-9-4-5-11-18(16)21(1

InchiKey: GUZBPGZOTDAWBO-UHFFFAOYSA-N

Formula: C21H13N

SMILES: c1ccc2nc3c4ccccc4c4ccccc4c3cc2c1

Mol. weight [g/mol]: 279.34

Physical Properties

Property code	Value	Unit	Source
hf	393.61	kJ/mol	Cheméo Relay (1.0)
hvap	133.20	kJ/mol	Cheméo Relay (1.0)
ie	7.69	eV	Cheméo Relay (1.0)
log10ws	-7.15		Cheméo Relay (1.0)
logp	5.694		Crippen Method
mcvol	215.130	ml/mol	McGowan Method
tb	783.10	K	Cheméo Relay (1.0)
tf	471.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.80	kJ/mol	477.40	NIST Webbook

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=C215623&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point