

9-PHENYLACRIDINE

Other names:	9-Phenylacridine
Inchi:	InChI=1S/C19H13N/c1-2-8-14(9-3-1)19-15-10-4-6-12-17(15)20-18-13-7-5-11-16(18)19/h
InchiKey:	MTRFEWTTWIPAXLG-UHFFFAOYSA-N
Formula:	C19H13N
SMILES:	c1ccc(-c2c3ccccc3nc3ccccc23)cc1
Mol. weight [g/mol]:	255.32

Physical Properties

Property code	Value	Unit	Source
af	0.5495		Cheméo Relay (1.0)
gf	423.66	kJ/mol	Cheméo Relay (1.0, beta)
hf	378.39	kJ/mol	Cheméo Relay (1.0)
hvap	111.52	kJ/mol	Cheméo Relay (1.0)
ie	7.75	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-5.83		Cheméo Relay (1.0)
logp	5.055		Crippen Method
mcvol	202.110	ml/mol	McGowan Method
pc	2887.70	kPa	Cheméo Relay (1.0, beta)
tb	705.34	K	Cheméo Relay (1.0)
tc	1027.70	K	Cheméo Relay (1.0)
tf	426.35	K	Cheméo Relay (1.0)
vc	0.752	m3/kmol	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C602562&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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

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