9,10,12-Trimethylbenz[a]acridine

Other names:	5,7,8-Trimethyl-3:4-benzacridine
	2,3,10 Trimethyl,5:6 benzacridine
	9,10,12-Trimethylbenz[a]acridine
Inchi:	InChI=1S/C20H17N/c1-12-10-17-14(3)20-16-7-5-4-6-15(16)8-9-18(20)21-19(17)11-13(12
InchiKey:	CWOZJMDRFAMWLF-UHFFFAOYSA-N
Formula:	C20H17N
SMILES:	Cc1cc2nc3ccc4ccccc4c3c(C)c2cc1C
Mol. weight [g/mol]:	271.36

Physical Properties

Property code	Value	Unit	Source
af	0.6317		Cheméo Relay (1.0)
hf	249.89	kJ/mol	Cheméo Relay (1.0)
ie	7.36	eV	Cheméo Relay (1.0)
log10ws	-6.80		Cheméo Relay (1.0)
logp	5.466		Crippen Method
mcvol	220.500	ml/mol	McGowan Method
pc	1991.28	kPa	Cheméo Relay (1.0, beta)
rinpol	466.79		NIST Webbook
rinpol	466.79		NIST Webbook
tb	725.34	K	Cheméo Relay (1.0)
tc	1041.39	K	Cheméo Relay (1.0)
tf	456.41	K	Cheméo Relay (1.0)
vc	0.832	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63040028&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

af:	Acentric Factor
hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume