EMDP

Inchi: InChI=1S/C19H21N/c1-3-18-19(14-15(2)20-18,16-10-6-4-7-11-16)17-12-8-5-9-13-17/h4-
InchiKey: UPZKJIHNKKJIKX-UHFFFAOYSA-N
Formula: C19H21N
SMILES: CCC1=NC(C)CC1(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 263.38
CAS: 102177-18-4

Physical Properties

Property code	Value	Unit	Source
gf	494.38	kJ/mol	Joback Method
hf	210.23	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.616		Crippen Method
mcvol	225.870	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	756.17	K	Joback Method
tc	1020.68	K	Joback Method
tf	472.11	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.21	J/mol×K	756.17	Joback Method
cpg	694.01	J/mol×K	800.25	Joback Method
cpg	714.49	J/mol×K	844.34	Joback Method
cpg	733.92	J/mol×K	888.42	Joback Method
cpg	752.55	J/mol×K	932.51	Joback Method
cpg	770.63	J/mol×K	976.59	Joback Method
cpg	788.41	J/mol×K	1020.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102177184&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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