N-Desmethylcyclobenzaprine

Inchi: InChI=1S/C19H19N/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16-8-3-5-10-18(16)19/h2-
InchiKey: XECQQDXTQRYYBH-UHFFFAOYSA-N
Formula: C19H19N
SMILES: CNCCC=C1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]: 261.36
CAS: 303-50-4

Physical Properties

Property code	Value	Unit	Source
gf	547.93	kJ/mol	Joback Method
hf	295.05	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.212		Crippen Method
mcvol	221.570	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2318.60		NIST Webbook
tb	764.82	K	Joback Method
tc	1004.07	K	Joback Method
tf	467.73	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.64	J/mol×K	764.82	Joback Method
cpg	635.75	J/mol×K	804.69	Joback Method
cpg	650.75	J/mol×K	844.57	Joback Method
cpg	664.76	J/mol×K	884.44	Joback Method
cpg	677.94	J/mol×K	924.32	Joback Method
cpg	690.41	J/mol×K	964.19	Joback Method
cpg	702.30	J/mol×K	1004.07	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=C303504&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