Cyclobenzaprine

Other names:	1-Propanamine, 3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl- 5H-Dibenzo(a,d)cycloheptene-«delta»5,«gamma»-propylamine, N,N-dimethyl- N,N-Dimethyl-5H-dibenzo(a,d)cycloheptene-«delta»5,«gamma»-propylamine 5-(3-Dimetilaminopropiliden)-5H-dibenzo-(a,d)-ciclopentene Proeptatriene Proheptatriene MK 130 Ro 4-1577 RP 9715 10,11-Dehydroamitriptyline 9715 R.P Proheptatrien 3-(5H-Dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine
Inchi:	InChI=1S/C20H21N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/
InchiKey:	JURKNVYFZMSNLP-UHFFFAOYSA-N
Formula:	C20H21N
SMILES:	CN(C)CCC=C1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]:	275.39
CAS:	303-53-7

Physical Properties

Property code	Value	Unit	Source
gf	577.74	kJ/mol	Joback Method
hf	288.47	kJ/mol	Joback Method
hfus	36.49	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.554		Crippen Method
mcvol	235.660	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	749.97	K	Joback Method
tc	983.67	K	Joback Method
tf	458.81	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.74	J/mol×K	749.97	Joback Method
cpg	677.08	J/mol×K	788.92	Joback Method
cpg	693.22	J/mol×K	827.87	Joback Method
cpg	708.31	J/mol×K	866.82	Joback Method
cpg	722.48	J/mol×K	905.77	Joback Method
cpg	735.88	J/mol×K	944.72	Joback Method
cpg	748.64	J/mol×K	983.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C303537&Units=SI
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

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

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