Protriptyline

Other names:	5H-Dibenzo[a,d]cycloheptene-5-propanamine, N-methyl- 5H-Dibenzo[a,d]cycloheptene-5-propylamine, N-methyl- Amimetilina MK 240 Protryptyline Triptil 5-(3-Methylaminopropyl)-5H-Dibenzo[a,d]cycloheptene 7-(3-Methylaminopropyl)-1,2:5,6-dibenzocycloheptatriene N-3-(5H-Dibenzo(a,d)cyclohepten-5-yl)propyl-N-methylamine N-Methyl-5H-dibenzo[a,d]cycloheptene-5-propylamine
Inchi:	InChI=1S/C19H21N/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:	BWPIARFWQZKAIA-UHFFFAOYSA-N
Formula:	C19H21N
SMILES:	CNCCCC1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]:	263.38
CAS:	438-60-8

Physical Properties

Property code	Value	Unit	Source
gf	494.76	kJ/mol	Joback Method
hf	198.68	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.302		Crippen Method
mcvol	225.870	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2319.20		NIST Webbook
rinpol	2251.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	2230.00		NIST Webbook

rinpol	2261.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2319.20		NIST Webbook
tb	753.51	K	Joback Method
tc	986.87	K	Joback Method
tf	453.13	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.24	J/mol×K	753.51	Joback Method
cpg	666.69	J/mol×K	792.40	Joback Method
cpg	682.91	J/mol×K	831.30	Joback Method
cpg	698.00	J/mol×K	870.19	Joback Method
cpg	712.09	J/mol×K	909.08	Joback Method
cpg	725.29	J/mol×K	947.97	Joback Method
cpg	737.71	J/mol×K	986.87	Joback Method

Sources

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=C438608&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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