Maprotiline

Other names:	9,10-Ethanoanthracene-9(10H)-propanamine, N-methyl- 9,10-Ethanoanthracene-9(10H)-propylamine, N-methyl- 276-Ba 3-(9,10-Dihydro-9,10-ethanoanthracen-9-yl)propylmethylamine Ludiomil Maprotylina N-Methyl-9,10-ethanoanthracene-9(10H)-propylamine
Inchi:	InChI=1S/C20H23N/c1-21-14-6-12-20-13-11-15(16-7-2-4-9-18(16)20)17-8-3-5-10-19(17)
InchiKey:	QSLMDECMDJKHMQ-UHFFFAOYSA-N
Formula:	C20H23N
SMILES:	CNCCCC12CCC(c3ccccc31)c1ccccc12
Mol. weight [g/mol]:	277.40
CAS:	10262-69-8

Physical Properties

Property code	Value	Unit	Source
gf	552.68	kJ/mol	Joback Method
hf	220.62	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.211		Crippen Method
mcvol	233.400	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2403.20		NIST Webbook
rinpol	2341.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	775.67	K	Joback Method
tc	1011.20	K	Joback Method

tf	512.52	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.91	J/mol×K	775.67	Joback Method
cpg	722.50	J/mol×K	814.93	Joback Method
cpg	740.58	J/mol×K	854.18	Joback Method
cpg	758.45	J/mol×K	893.44	Joback Method
cpg	776.39	J/mol×K	932.69	Joback Method
cpg	794.69	J/mol×K	971.95	Joback Method
cpg	813.64	J/mol×K	1011.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10262698&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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