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]: 277.41

Physical Properties

Property code	Value	Unit	Source
hfus	34.13	kJ/mol	Joback Method
logp	4.211		Crippen Method
mcvol	233.400	ml/mol	McGowan Method
rinpol	2296.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2341.00		NIST Webbook
rinpol	2403.20		NIST Webbook
rinpol	2381.00		NIST Webbook

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10262698&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices