BENZOCTAMINE

Other names:	Benzoctamine
	Benzoktamina
	Tacitin
	N-Methyl-9,10-ethanoanthracene-9(10H)-methylamine
	N-Methyl-9,10-ethanoantrhacene-9(10H)-methylamine
Inchi:	InChI=1S/C18H19N/c1-19-12-18-11-10-13(14-6-2-4-8-16(14)18)15-7-3-5-9-17(15)18/h2-
InchiKey:	GNRXCIONJWKSEA-UHFFFAOYSA-N
Formula:	C18H19N
SMILES:	CNCC12CCC(c3ccccc31)c1ccccc12
Mol. weight [g/mol]:	249.36

Physical Properties

Property code	Value	Unit	Source
hfus	28.95	kJ/mol	Joback Method
logp	3.431		Crippen Method
mcvol	205.220	ml/mol	McGowan Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.07	J/mol×K	729.91	Joback Method
cpg	610.63	J/mol×K	770.72	Joback Method
cpg	627.48	J/mol×K	811.54	Joback Method
cpg	643.92	J/mol×K	852.35	Joback Method
cpg	660.28	J/mol×K	893.16	Joback Method
cpg	676.86	J/mol×K	933.97	Joback Method
cpg	693.98	J/mol×K	974.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17243399&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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