

9,10-Ethanoanthracene-9(10H)-methylamine, N-methyl-, 9,10-dihydro

Other names:

Benzoctamine

Benzoktamina

Tacitin

N-Methyl-9,10-ethanoanthracene-9(10H)-methylamine

N-Methyl-9,10-ethanoanthracene-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(c3cccc31)c1cccc12

Mol. weight [g/mol]:

249.35

CAS:

17243-39-9

Physical Properties

Property code	Value	Unit	Source
gf	535.84	kJ/mol	Joback Method
hf	261.90	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.431		Crippen Method
mcvol	205.220	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	729.91	K	Joback Method
tc	974.79	K	Joback Method
tf	489.98	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.07	J/molxK	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17243399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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