

2,3,3-TRIMETHYLINDOLENINE

Other names:	2,3,3-Trimethyl-3H-indole 2,3,3-Trimethylindolenine
Inchi:	InChI=1S/C11H13N/c1-8-11(2,3)9-6-4-5-7-10(9)12-8/h4-7H,1-3H3
InchiKey:	FLHJIAFUWHPJRT-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	CC1=Nc2ccccc2C1(C)C
Mol. weight [g/mol]:	159.23

Physical Properties

Property code	Value	Unit	Source
hfus	15.71	kJ/mol	Joback Method
logp	3.070		Crippen Method
mcvol	136.910	ml/mol	McGowan Method
tb	501.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.93	J/mol×K	547.56	Joback Method
cpg	345.19	J/mol×K	587.98	Joback Method
cpg	360.25	J/mol×K	628.40	Joback Method
cpg	374.29	J/mol×K	668.82	Joback Method
cpg	387.46	J/mol×K	709.24	Joback Method
cpg	399.96	J/mol×K	749.66	Joback Method
cpg	411.94	J/mol×K	790.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	501.70	K	99.20	NIST Webbook

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=C1640397&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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