N-methyl-3,4-methylenedioxyamphetamine

Other names:	MDMA
	Ecstasy
	Adam
	1,3-Benzodioxole-5-ethanamine, N,«alpha»-dimethyl-
	XTC
	3,4-Methylenedioxymethamphetamine
	3,4-Methylenedioxymethylamphetamine
	Methamphetamine, 3,4-methylenedioxy
	Methylenedioxymethamphetamine
	(RS)-3,4-(Methylenedioxy)methamphetamine
	3,4-Methylenedioxy-N,«alpha»-dimethyl-«beta»-phenylethylamine
	DL-(3,4-Methylenedioxy)methamphetamine
	Phenethylamine, N,«alpha»-dimethyl-3,4-methylenedioxy-
	(.+/-.)-(3,4-Methylenedioxy)methamphetamine
	64057-70-1 (hydrochloride)
	methylenedioxymetamphetamine (MDMA,XTC)
	Methylenedioxymethamphetamine (MDMA)
Inchi:	InChI=1S/C11H15NO2/c1-8(12-2)5-9-3-4-10-11(6-9)14-7-13-10/h3-4,6,8,12H,5,7H2,1-2H
InchiKey:	SHXWCVYOXRDMCX-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CNC(C)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	193.25

Physical Properties

Property code	Value	Unit	Source
hfus	32.11	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
logp	1.566		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
rinpol	1553.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1551.10		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1553.00		NIST Webbook

rinpol	1551.10		NIST Webbook
tb	543.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.82	J/mol×K	602.76	Joback Method
cpg	410.43	J/mol×K	639.67	Joback Method
cpg	424.06	J/mol×K	676.58	Joback Method
cpg	436.78	J/mol×K	713.49	Joback Method
cpg	448.65	J/mol×K	750.40	Joback Method
cpg	459.75	J/mol×K	787.31	Joback Method
cpg	470.13	J/mol×K	824.22	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42542109&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature