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]:	193.24
CAS:	42542-10-9

Physical Properties

Property code	Value	Unit	Source
gf	118.06	kJ/mol	Joback Method
hf	-179.45	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.566		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1551.10		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook

rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1551.10		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	602.76	K	Joback Method
tc	824.22	K	Joback Method
tf	378.17	K	Joback Method
vc	0.573	m3/kmol	Joback Method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42542109&Units=SI

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