Tenamfetamine

Other names:	3,4-Methylenedioxy-amphetamine
	MDA
	Phenethylamine, «alpha»-methyl-3,4-(methylenedioxy)-
	1,3-Benzodioxole-5-ethanamine, «alpha»-methyl-
	Methylenedioxyamphetamine
	«alpha»-Methyl-3,4-(methylenedioxy)phenethylamine
	(.+/-.)-3,4-Methylenedioxyamphetamine
Inchi:	InChI=1S/C10H13NO2/c1-7(11)4-8-2-3-9-10(5-8)13-6-12-9/h2-3,5,7H,4,6,11H2,1H3
InchiKey:	NGBBVGZWCFBOGO-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(N)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	179.22
CAS:	51497-09-7

Physical Properties

Property code	Value	Unit	Source
gf	86.70	kJ/mol	Joback Method
hf	-178.49	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	60.95	kJ/mol	Joback Method
ie	8.01 ± 0.06	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	1.305		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	602.24	K	Joback Method
tc	836.85	K	Joback Method
tf	397.50	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.51	J/mol×K	602.24	Joback Method

cpg	371.07	J/mol×K	641.34	Joback Method
cpg	383.66	J/mol×K	680.44	Joback Method
cpg	395.34	J/mol×K	719.55	Joback Method
cpg	406.20	J/mol×K	758.65	Joback Method
cpg	416.30	J/mol×K	797.75	Joback Method
cpg	425.71	J/mol×K	836.85	Joback Method

Sources

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=C51497097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume