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:	4764-17-4

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
log10ws	-2.45		Crippen Method
logp	1.305		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1508.80		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1472.00		NIST Webbook

rinpol	1434.00		NIST Webbook
rinpol	1480.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2204.00		NIST Webbook
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=C4764174&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume