3,4-Methylenedioxy-2-methoxyamphetamine

Other names: Methoxymethylenedioxyamphetamine
Inchi: InChI=1S/C11H15NO3/c1-7(12)5-8-3-4-9-11(10(8)13-2)15-6-14-9/h3-4,7H,5-6,12H2,1-2H
InchiKey: OSJXZWMDUMAITM-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: COc1c(CC(C)N)ccc2c1OCO2
Mol. weight [g/mol]: 209.24
CAS: 23693-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-19.51	kJ/mol	Joback Method
hf	-342.82	kJ/mol	Joback Method
hfus	33.00	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.314		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	652.52	K	Joback Method
tc	880.18	K	Joback Method
tf	443.52	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.40	J/mol×K	652.52	Joback Method
cpg	443.14	J/mol×K	690.46	Joback Method
cpg	456.00	J/mol×K	728.41	Joback Method
cpg	468.02	J/mol×K	766.35	Joback Method
cpg	479.25	J/mol×K	804.30	Joback Method
cpg	489.74	J/mol×K	842.24	Joback Method

cpg	499.52	J/mol×K	880.18	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=C23693198&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