3-Methoxymethamphetamine

Other names: Methamphetamine, 3-methoxy
Inchi: InChI=1S/C11H17NO/c1-9(12-2)7-10-5-4-6-11(8-10)13-3/h4-6,8-9,12H,7H2,1-3H3
InchiKey: USQWRDRXXKZFDI-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: CNC(C)Cc1cccc(OC)c1
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
gf	126.47	kJ/mol	Joback Method
hf	-129.34	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.846		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
tb	554.89	K	Joback Method
tc	761.71	K	Joback Method
tf	312.56	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.82	J/mol×K	554.89	Joback Method
cpg	392.50	J/mol×K	589.36	Joback Method
cpg	407.36	J/mol×K	623.83	Joback Method
cpg	421.41	J/mol×K	658.30	Joback Method
cpg	434.67	J/mol×K	692.77	Joback Method
cpg	447.17	J/mol×K	727.24	Joback Method
cpg	458.92	J/mol×K	761.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U335169&Units=SI
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

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