N-Methyl-N-trifluoroacetyl-3,4-methylenedioxyam

Other names: MDMA N-TFA
MDMA, TFA
Methylenedioxyamphetamine N-TFA
Inchi: InChI=1S/C13H14F3NO3/c1-8(17(2)12(18)13(14,15)16)5-9-3-4-10-11(6-9)20-7-19-10/h3
InchiKey: KACKAPXORIPDQB-UHFFFAOYSA-N
Formula: C13H14F3NO3
SMILES: CC(Cc1ccc2c(c1)OCO2)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 289.25
CAS: 158097-59-7

Physical Properties

Property code	Value	Unit	Source
gf	-554.22	kJ/mol	Joback Method
hf	-916.33	kJ/mol	Joback Method
hfus	38.63	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.367		Crippen Method
mcvol	188.010	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	659.24	K	Joback Method
tc	861.44	K	Joback Method
tf	434.64	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.47	J/mol×K	659.24	Joback Method
cpg	539.94	J/mol×K	692.94	Joback Method
cpg	552.43	J/mol×K	726.64	Joback Method
cpg	564.03	J/mol×K	760.34	Joback Method
cpg	574.82	J/mol×K	794.04	Joback Method
cpg	584.88	J/mol×K	827.74	Joback Method

cpg	594.29	J/mol×K	861.44	Joback Method

Sources

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=C158097597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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