p-Nitromethylamphetamine

Inchi: InChI=1S/C10H14N2O2/c1-8(11-2)7-9-3-5-10(6-4-9)12(13)14/h3-6,8,11H,7H2,1-2H3
InchiKey: FMYSLOHXMJLTRT-UHFFFAOYSA-N
Formula: C10H14N2O2
SMILES: CNC(C)Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	258.60	kJ/mol	Joback Method
hf	12.76	kJ/mol	Joback Method
hfus	28.25	kJ/mol	Joback Method
hvap	63.43	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	1.745		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	661.43	K	Joback Method
tc	898.78	K	Joback Method
tf	422.67	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.30	J/mol×K	661.43	Joback Method
cpg	421.22	J/mol×K	700.99	Joback Method
cpg	434.14	J/mol×K	740.55	Joback Method
cpg	446.09	J/mol×K	780.10	Joback Method
cpg	457.13	J/mol×K	819.66	Joback Method
cpg	467.31	J/mol×K	859.22	Joback Method
cpg	476.68	J/mol×K	898.78	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=R18272&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume