2,4,6-Trimethylnitrosobenzene

Inchi: InChI=1S/C9H11NO/c1-6-4-7(2)9(10-11)8(3)5-6/h4-5H,1-3H3
InchiKey: FEKDDEQYKDNKJG-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: Cc1cc(C)c(N=O)c(C)c1
Mol. weight [g/mol]: 149.19
CAS: 1196-12-9

Physical Properties

Property code	Value	Unit	Source
hf	107.40 ± 1.90	kJ/mol	NIST Webbook
hvap	48.99	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.010		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	510.34	K	Joback Method
tc	718.78	K	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=C1196129&Units=SI

Legend

hf: Enthalpy of formation 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