neo-Pentyl nitrite

Other names: Nitrous acid, 2,2-dimethylpropyl ester
Inchi: InChI=1S/C5H11NO2/c1-5(2,3)4-8-6-7/h4H2,1-3H3
InchiKey: YIGAWISCEHGPRK-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CC(C)(C)CON=O
Mol. weight [g/mol]: 117.15

Physical Properties

Property code	Value	Unit	Source
hf	-455.69	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.731		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	578.00		NIST Webbook
rinpol	585.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	585.00		NIST Webbook
ripol	750.00		NIST Webbook
ripol	750.00		NIST Webbook
tb	396.39	K	Joback Method
tc	575.61	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120224&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature