C2H5C(CH3)2ONO

Other names: tert.-Pentyl nitrite
Inchi: InChI=1S/C5H11NO2/c1-4-5(2,3)8-6-7/h4H2,1-3H3
InchiKey: JXCNBASKFCBVAN-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CCC(C)(C)ON=O
Mol. weight [g/mol]: 117.15
CAS: 5156-41-2

Physical Properties

Property code	Value	Unit	Source
hf	-192.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-251.00	kJ/mol	NIST Webbook
hvap	59.80	kJ/mol	NIST Webbook
log10ws	-2.30		Crippen Method
logp	1.873		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	621.00		NIST Webbook
rinpol	621.00		NIST Webbook
ripol	815.00		NIST Webbook
ripol	815.00		NIST Webbook
tb	396.39	K	Joback Method
tc	575.61	K	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=C5156412&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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