2-Pentyl nitrite

Other names: CH3(CH2)2CH(CH3)ONO
Inchi: InChI=1S/C5H11NO2/c1-3-4-5(2)8-6-7/h5H,3-4H2,1-2H3
InchiKey: PPCIUPZUHKICQG-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CCCC(C)ON=O
Mol. weight [g/mol]: 117.15
CAS: 5145-25-5

Physical Properties

Property code	Value	Unit	Source
hf	-452.22	kJ/mol	Joback Method
hvap	37.84	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.873		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	646.00		NIST Webbook
rinpol	646.00		NIST Webbook
ripol	825.00		NIST Webbook
ripol	825.00		NIST Webbook
tb	399.18	K	Joback Method
tc	571.22	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5145255&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

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