Heptyl nitrite

Inchi: InChI=1S/C7H15NO2/c1-2-3-4-5-6-7-10-8-9/h2-7H2,1H3
InchiKey: IAHLQSRLEFUEMK-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CCCCCCCON=O
Mol. weight [g/mol]: 145.20

Physical Properties

Property code	Value	Unit	Source
hf	-488.22	kJ/mol	Joback Method
hvap	42.68	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.655		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	445.38	K	Joback Method
tc	611.98	K	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=R311529&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/96-937-6/Heptyl-nitrite.pdf
Generated by Cheméo on 2024-04-29 07:18:42.471171842 +0000 UTC m=+16664371.391749153.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.