

Hexyl nitrite

Inchi: InChI=1S/C6H13NO2/c1-2-3-4-5-6-9-7-8/h2-6H2,1H3
InchiKey: SGRWGISGVDVSJV-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CCCCCCON=O
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
hf	-467.58	kJ/mol	Joback Method
hvap	40.46	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.265		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	422.50	K	Joback Method
tc	589.98	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=R311534&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

Latest version available from:

<https://www.chemeo.com/cid/98-497-3/Hexyl-nitrite.pdf>

Generated by Cheméo on 2024-04-28 00:29:56.4510014 +0000 UTC m=+16553445.371578715.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.