

2-heptadecanone O-methyloxime

Inchi: InChI=1S/C18H37NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2)19-20-3/h4-17H2,1-
InchiKey: SHPYNUARUZVYGM-VHEBQXMUSA-N
Formula: C18H37NO
SMILES: CCCCCCCCCCCCCCCC(C)=NOC
Mol. weight [g/mol]: 283.49

Physical Properties

Property code	Value	Unit	Source
hf	-474.64	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.490		Crippen Method
mcvol	276.030	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
ripol	2827.00		NIST Webbook
ripol	2827.00		NIST Webbook
tb	710.22	K	Joback Method
tc	885.54	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R320360&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/89-085-0/2-heptadecanone-O-methyloxime.pdf>

Generated by Cheméo on 2024-04-27 02:11:33.773926283 +0000 UTC m=+16473142.694503595.

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