N-heptaldoxime

Other names: heptanal oxime
Inchi: InChI=1S/C7H15NO/c1-2-3-4-5-6-7-8-9/h7,9H,2-6H2,1H3/b8-7+
InchiKey: BNYNJIKGRPHFAM-BQYQJAHWSA-N
Formula: C7H15NO
SMILES: CCCCCCC=NO
Mol. weight [g/mol]: 129.20
CAS: 629-31-2

Physical Properties

Property code	Value	Unit	Source
hf	-257.82	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	2.417		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
tb	468.20	K	NIST Webbook
tc	705.99	K	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.70	K	1.90	NIST Webbook

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=C629312&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature