Octanone-4-oxime

Inchi:	InChI=1S/C8H17NO/c1-3-5-7-8(9-10)6-4-2/h10H,3-7H2,1-2H3/b9-8+
InchiKey:	AKLMPECUKBNPII-CMDGGOBGSA-N
Formula:	C8H17NO
SMILES:	CCCCC(CCC)=NO
Mol. weight [g/mol]:	143.23
CAS:	7207-51-4

Physical Properties

Property code	Value	Unit	Source
chl	-5339.40 ± 1.80	kJ/mol	NIST Webbook
hf	-181.10 ± 3.70	kJ/mol	NIST Webbook
hvap	53.48	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.807		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
tb	551.18	K	Joback Method
tc	729.99	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	68.80	kJ/mol	346.50	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=C7207514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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