2,3-Octanedione 3-oxime

Inchi: InChI=1S/C8H15NO2/c1-3-4-5-6-8(9-11)7(2)10/h11H,3-6H2,1-2H3/b9-8+
InchiKey: CVRXVGUWTKLMFD-CMDGGOBGSA-N
Formula: C8H15NO2
SMILES: CCCCCC(=NO)C(C)=O
Mol. weight [g/mol]: 157.21
CAS: 584-92-9

Physical Properties

Property code	Value	Unit	Source
hf	-400.83	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.986		Crippen Method
mcvol	136.700	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	605.05	K	Joback Method
tc	791.76	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=C584929&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

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