

Butanal, oxime

Other names:	Butyraldehyde, oxime n-Butyraldoxime Butylaldoxime Butyraldoxime CH3(CH2)2CH=NOH n-Butyraldehyde, oxime USAF AM-6 Exkin 1 Exkin No. 1 anti-skinning agent Skino No. 1 Troykyd anti-skin bto UN 2840 Butanaldoxime n-Butylaldoxime NSC 1487
Inchi:	InChI=1S/C4H9NO/c1-2-3-4-5-6/h4,6H,2-3H2,1H3
InchiKey:	KGGVGTQEGGOZRN-UHFFFAOYSA-N
Formula:	C4H9NO
SMILES:	CCCC=NO
Mol. weight [g/mol]:	87.12
CAS:	110-69-0

Physical Properties

Property code	Value	Unit	Source
hf	-195.90	kJ/mol	Joback Method
hvap	44.49	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.93	eV	NIST Webbook
log10ws	-0.31		Crippen Method
logp	1.246		Crippen Method
mcvol	78.770	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	793.00		NIST Webbook
tb	459.78	K	Joback Method
tc	642.49	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	55.80	kJ/mol	328.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.20	K	95.30	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=C110690&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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