2-Butanone, 3-methyl-3-nitroso-, dimer

Inchi:	InChI=1S/2C5H9NO2/c2*1-4(7)5(2,3)6-8/h2*1-3H3
InchiKey:	OESDVLGRNFMZSQ-UHFFFAOYSA-N
Formula:	C10H18N2O4
SMILES:	CC(=O)C(C)(C)N=O.CC(=O)C(C)(C)N=O
Mol. weight [g/mol]:	230.26
CAS:	30442-79-6

Physical Properties

Property code	Value	Unit	Source
hf	-940.39	kJ/mol	Joback Method
hvap	67.24	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.241		Crippen Method
mcvol	188.860	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
tb	657.68	K	Joback Method
tc	860.37	K	Joback Method

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=C30442796&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
tc:	Critical Temperature

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