

2-Nonen-4-one, 2-methyl-

Other names:	2-Methyl-2-nonen-4-one 2-methylnon-2-en-4-one
Inchi:	InChI=1S/C10H18O/c1-4-5-6-7-10(11)8-9(2)3/h8H,4-7H2,1-3H3
InchiKey:	LVVHLEIGMGTYJL-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CCCCC(=O)C=C(C)C
Mol. weight [g/mol]:	154.25
CAS:	2903-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.93	kJ/mol	Joback Method
hf	-254.88	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mvol	149.030	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1215.00		NIST Webbook
tb	486.11	K	Joback Method
tc	669.94	K	Joback Method
tf	233.35	K	Joback Method
vc	0.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.17	J/mol×K	486.11	Joback Method
cpg	339.51	J/mol×K	516.75	Joback Method
cpg	353.18	J/mol×K	547.39	Joback Method
cpg	366.21	J/mol×K	578.03	Joback Method
cpg	378.61	J/mol×K	608.66	Joback Method
cpg	390.41	J/mol×K	639.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2903233&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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