

2-Cyclohexen-1-one, 3,6,6-trimethyl-

Other names:	3,6,6-Trimethyl-2-cyclohexen-1-one
Inchi:	InChI=1S/C9H14O/c1-7-4-5-9(2,3)8(10)6-7/h6H,4-5H2,1-3H3
InchiKey:	DKUDUXARZQESDM-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1=CC(=O)C(C)(C)CC1
Mol. weight [g/mol]:	138.21
CAS:	23438-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-58.40	kJ/mol	Joback Method
hf	-250.92	kJ/mol	Joback Method
hfus	4.95	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	497.07	K	Joback Method
tc	727.23	K	Joback Method
tf	303.97	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.69	J/mol×K	497.07	Joback Method
cpg	291.98	J/mol×K	535.43	Joback Method
cpg	307.32	J/mol×K	573.79	Joback Method
cpg	321.80	J/mol×K	612.15	Joback Method
cpg	335.52	J/mol×K	650.51	Joback Method

cpg	348.57	J/mol×K	688.87	Joback Method
cpg	361.03	J/mol×K	727.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	2.00	NIST Webbook

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=C23438779&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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