

2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-,

Other names: (1Z)-1-(3,5,5-Trimethyl-2-cyclohexen-1-ylidene)-2-propanone
cis-2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-

Inchi: InChI=1S/C12H18O/c1-9-5-11(6-10(2)13)8-12(3,4)7-9/h5-6H,7-8H2,1-4H3/b11-6+

InchiKey: BPMFQXXZWSBLRP-IZZDOVSWSA-N

Formula: C12H18O

SMILES: CC(=O)C=C1C=C(C)CC(C)(C)C1

Mol. weight [g/mol]: 178.27

CAS: 16695-73-1

Physical Properties

Property code	Value	Unit	Source
gf	5.99	kJ/mol	Joback Method
hf	-211.69	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.268		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1436.00		NIST Webbook
tb	558.40	K	Joback Method
tc	777.62	K	Joback Method
tf	329.85	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.95	J/molxK	558.40	Joback Method
cpg	404.87	J/molxK	594.94	Joback Method
cpg	420.78	J/molxK	631.47	Joback Method
cpg	435.79	J/molxK	668.01	Joback Method
cpg	450.03	J/molxK	704.55	Joback Method
cpg	463.61	J/molxK	741.09	Joback Method

Sources

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=C16695731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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