

2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)-, (S)-

Other names:	p-Menth-6-en-2-one, (S)-(+)- (+)-Carvotanacetone Carvotanacetone, (+)- Carvotanacetone Carvotanacetone
Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,7,9H,5-6H2,1-3H3/t9-/m1/s1
InchiKey:	WPGPCDVQHXOMQP-SECBINFHSA-N
Formula:	C10H16O
SMILES:	CC1=CCC(C(C)C)CC1=O
Mol. weight [g/mol]:	152.23
CAS:	499-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-46.93	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1250.20		NIST Webbook
rinpol	1250.20		NIST Webbook

ripol	1247.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	519.27	K	Joback Method
tc	741.04	K	Joback Method
tf	276.34	K	Joback Method
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.40	J/mol×K	519.27	Joback Method
cpg	339.21	J/mol×K	556.23	Joback Method
cpg	356.17	J/mol×K	593.19	Joback Method
cpg	372.28	J/mol×K	630.16	Joback Method
cpg	387.53	J/mol×K	667.12	Joback Method
cpg	401.93	J/mol×K	704.08	Joback Method
cpg	415.47	J/mol×K	741.04	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=C499718&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
hvac:	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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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