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

Other names: p-Menth-6-en-2-one, (S)-(+)-
(+)-Carvotanacetone
Carvotanacetone, (+)-
Carvotanacetone
Carvotanaceton

Inchi: InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,7,9H,5-6H2,1-3H3/t9-/m0/s1

InchiKey: WPGPCDVQHXOMQP-SECBINFHSA-N

Formula: C10H16O

SMILES: CC1=CC[C@H](C(C)C)CC1=O

Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
hf	-218.42	kJ/mol	Cheméo Relay (1.0)
hfus	10.31	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Cheméo Relay (1.0)
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1218.00		NIST Webbook
rinpol	1250.20		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1250.20		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1256.00		NIST Webbook

rinpol	1256.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1697.00		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
ripol	1716.00		NIST Webbook
tb	488.06	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C499718&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature