

3-Cyclohexen-1-one, 2-isopropyl-5-methyl-

Other names:	2-Isopropyl-5-methyl-3-cyclohexen-1-one 2-Isopropyl-5-methylcyclohex-3-en-1-one
Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h4-5,7-9H,6H2,1-3H3
InchiKey:	GPUOMCZFJZZLJT-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1C=CC(C(C)C)C(=O)C1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-45.01	kJ/mol	Joback Method
hf	-300.95	kJ/mol	Joback Method
hfus	11.77	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1251.00		NIST Webbook
tb	509.62	K	Joback Method
tc	730.05	K	Joback Method
tf	259.58	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.62	J/mol×K	509.62	Joback Method
cpg	340.19	J/mol×K	546.36	Joback Method
cpg	357.89	J/mol×K	583.10	Joback Method
cpg	374.70	J/mol×K	619.84	Joback Method

cpg	390.63	J/mol×K	656.58	Joback Method
cpg	405.65	J/mol×K	693.32	Joback Method
cpg	419.78	J/mol×K	730.05	Joback Method

Sources

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=U155470&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
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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