3-Cyclohexen-1-one, 3,5,5-trimethyl-

Other names:	«beta»-Isophorone
	«beta»-Phorone
	3,5,5-Trimethyl-3-cyclohexene-1-one
	3,5,5-Trimethylcyclohex-3-en-1-one
	3,5,5-trimethyl-3-cyclohexen-1-one
	3,5,5-Trimethylcyclohex-3-enone
Inchi:	InChI=1S/C9H14O/c1-7-4-8(10)6-9(2,3)5-7/h5H,4,6H2,1-3H3
InchiKey:	LKOKKQDYMZUSCG-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1=CC(C)(C)CC(=O)C1
Mol. weight [g/mol]:	138.21
CAS:	471-01-2

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	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1042.50		NIST Webbook
rinpol	1042.50		NIST Webbook
rinpol	1044.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1420.00		NIST Webbook

ripol	1408.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1416.00		NIST Webbook
tb	497.07	K	Joback Method
tc	727.23	K	Joback Method
tf	303.97	K	Joback Method
vc	0.464	m3/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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C471012&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume