4-Isopropyl-6-methyltetral-1-one

Other names:	4-Isopropyl-6-methyl-1,2,3,4-tetrahydronaphthalen-1-one
	10-nor-Calamenen-10-one
	4-Isopropyl-6-methyl-1-tetralone
	4-Isopropyl-6-methyltetralone
	4-Isopropyl-6-methyl-1,2,3,4-tetrahydronaphthalenone
Inchi:	InChI=1S/C14H18O/c1-9(2)11-6-7-14(15)12-5-4-10(3)8-13(11)12/h4-5,8-9,11H,6-7H2,1-
InchiKey:	KIZXBPVAPQXAMH-UHFFFAOYSA-N
Formula:	C14H18O
SMILES:	Cc1ccc2c(c1)C(C(C)C)CCC2=O
Mol. weight [g/mol]:	202.29
CAS:	57494-10-7

Physical Properties

Property code	Value	Unit	Source
gf	83.77	kJ/mol	Joback Method
hf	-195.04	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.711		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2419.00		NIST Webbook

tb	634.75	K	Joback Method
tc	870.27	K	Joback Method
tf	366.64	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.33	J/mol×K	634.75	Joback Method
cpg	484.30	J/mol×K	674.00	Joback Method
cpg	502.07	J/mol×K	713.26	Joback Method
cpg	518.66	J/mol×K	752.51	Joback Method
cpg	534.11	J/mol×K	791.77	Joback Method
cpg	548.44	J/mol×K	831.02	Joback Method
cpg	561.69	J/mol×K	870.27	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=C57494107&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