2,2,5,5-Tetramethyl-3-hexanone

Other names: Neopentyl t-butyl ketone
Inchi: InChI=1S/C10H20O/c1-9(2,3)7-8(11)10(4,5)6/h7H2,1-6H3
InchiKey: XUXJQANAPZHLMK-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CC(C)(C)CC(=O)C(C)(C)C
Mol. weight [g/mol]: 156.27
CAS: 868-91-7

Physical Properties

Property code	Value	Unit	Source
chl	-6350.70 ± 2.30	kJ/mol	NIST Webbook
gf	-89.92	kJ/mol	Joback Method
hf	-393.90 ± 2.30	kJ/mol	NIST Webbook
hfl	-442.70 ± 2.30	kJ/mol	NIST Webbook
hfus	8.43	kJ/mol	Joback Method
hvap	48.79	kJ/mol	NIST Webbook
hvap	48.80 ± 0.20	kJ/mol	NIST Webbook
hvap	48.79 ± 0.19	kJ/mol	NIST Webbook
log10ws	-2.81		Crippen Method
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	436.00 ± 4.00	K	NIST Webbook
tb	434.00 ± 4.00	K	NIST Webbook
tc	670.36	K	Joback Method
tf	257.23	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.18	J/mol×K	475.61	Joback Method
cpg	422.43	J/mol×K	637.90	Joback Method
cpg	409.18	J/mol×K	605.44	Joback Method

cpg	395.09	J/mol×K	572.98	Joback Method
cpg	380.09	J/mol×K	540.53	Joback Method
cpg	364.13	J/mol×K	508.07	Joback Method
cpg	434.87	J/mol×K	670.36	Joback Method
dvisc	0.0002645	Pa×s	475.61	Joback Method
dvisc	0.0003734	Pa×s	439.21	Joback Method
dvisc	0.0005610	Pa×s	402.82	Joback Method
dvisc	0.0009140	Pa×s	366.42	Joback Method
dvisc	0.0016583	Pa×s	330.02	Joback Method
dvisc	0.0034877	Pa×s	293.63	Joback Method
dvisc	0.0090525	Pa×s	257.23	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=C868917&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume