

Neopentyl ethyl ketone

Other names:	5,5-dimethyl-3-hexanone
Inchi:	InChI=1S/C8H16O/c1-5-7(9)6-8(2,3)4/h5-6H2,1-4H3
InchiKey:	BARYVXFFVQIMLI-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCC(=O)CC(C)(C)C
Mol. weight [g/mol]:	128.21
CAS:	5340-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-109.60	kJ/mol	Joback Method
hf	-329.78	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	433.08	K	Joback Method
tc	619.80	K	Joback Method
tf	232.27	K	Joback Method
vc	0.478	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.73	J/mol×K	433.08	Joback Method
cpg	320.09	J/mol×K	588.68	Joback Method
cpg	308.91	J/mol×K	557.56	Joback Method
cpg	297.11	J/mol×K	526.44	Joback Method
cpg	284.66	J/mol×K	495.32	Joback Method
cpg	271.54	J/mol×K	464.20	Joback Method
cpg	330.68	J/mol×K	619.80	Joback Method
dvisc	0.0003081	Paxs	433.08	Joback Method

dvisc	0.0004158	Paxs	399.61	Joback Method
dvisc	0.0005927	Paxs	366.14	Joback Method
dvisc	0.0009076	Paxs	332.67	Joback Method
dvisc	0.0015286	Paxs	299.21	Joback Method
dvisc	0.0029357	Paxs	265.74	Joback Method
dvisc	0.0068051	Paxs	232.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5340307&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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