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

Physical Properties

Property code	Value	Unit	Source
af	0.3826		Cheméo Relay (1.0)
gf	-109.60	kJ/mol	Joback Method
hf	-364.55	kJ/mol	Cheméo Relay (1.0)
hfus	10.66	kJ/mol	Joback Method
hvap	40.71	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	417.94	K	Cheméo Relay (1.0)
tc	597.20	K	Cheméo Relay (1.0)
tf	286.47	K	Cheméo Relay (1.0)
vc	0.445	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0068051	Pa×s	232.27	Joback Method
dvisc	0.0029357	Pa×s	265.74	Joback Method
dvisc	0.0015286	Pa×s	299.21	Joback Method
dvisc	0.0009076	Pa×s	332.67	Joback Method
dvisc	0.0005927	Pa×s	366.14	Joback Method
dvisc	0.0004158	Pa×s	399.61	Joback Method
dvisc	0.0003081	Pa×s	433.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5340307&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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