

Neopentyl isobutyl ketone

Other names:	2,2,6-trimethyl-4-heptanone
Inchi:	InChI=1S/C10H20O/c1-8(2)6-9(11)7-10(3,4)5/h8H,6-7H2,1-5H3
InchiKey:	YTMAMXJFGGHEGY-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(C)CC(=O)CC(C)(C)C
Mol. weight [g/mol]:	156.27
CAS:	40239-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-95.20	kJ/mol	Joback Method
hf	-376.34	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	478.40	K	Joback Method
tc	665.58	K	Joback Method
tf	239.81	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.76	J/molxK	478.40	Joback Method
cpg	360.79	J/molxK	509.60	Joback Method
cpg	376.01	J/molxK	540.79	Joback Method
cpg	390.45	J/molxK	571.99	Joback Method
cpg	404.14	J/molxK	603.18	Joback Method
cpg	417.12	J/molxK	634.38	Joback Method
cpg	429.40	J/molxK	665.58	Joback Method
dvisc	0.0101417	Paxs	239.81	Joback Method

dvisc	0.0035358	Paxs	279.57	Joback Method
dvisc	0.0016026	Paxs	319.34	Joback Method
dvisc	0.0008655	Paxs	359.11	Joback Method
dvisc	0.0005286	Paxs	398.87	Joback Method
dvisc	0.0003530	Paxs	438.63	Joback Method
dvisc	0.0002521	Paxs	478.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40239198&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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