5-Nonanone, 2,8-dimethyl-

Other names:	2,8-Dimethyl-5-nonanone
	Isoamyl ketone
	2,8-dimethylnonan-5-one
Inchi:	InChI=1S/C11H22O/c1-9(2)5-7-11(12)8-6-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	JQCWLRHNAHIIGW-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CC(C)CCC(=O)CCC(C)C
Mol. weight [g/mol]:	170.29
CAS:	2050-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-92.06	kJ/mol	Joback Method
hf	-393.51	kJ/mol	Joback Method
hfus	18.80	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.428		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
ripol	1529.00		NIST Webbook
tb	497.00 ± 5.00	K	NIST Webbook
tc	682.49	K	Joback Method
tf	233.66	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.60	J/mol×K	504.07	Joback Method
cpg	461.88	J/mol×K	652.75	Joback Method
cpg	448.52	J/mol×K	623.02	Joback Method
cpg	434.53	J/mol×K	593.28	Joback Method
cpg	419.89	J/mol×K	563.54	Joback Method

cpg	404.59	J/mol×K	533.81	Joback Method
cpg	474.62	J/mol×K	682.49	Joback Method
dvisc	0.0002241	Pa×s	504.07	Joback Method
dvisc	0.0003102	Pa×s	459.00	Joback Method
dvisc	0.0004607	Pa×s	413.93	Joback Method
dvisc	0.0007538	Pa×s	368.87	Joback Method
dvisc	0.0014145	Pa×s	323.80	Joback Method
dvisc	0.0032535	Pa×s	278.73	Joback Method
dvisc	0.0103191	Pa×s	233.66	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=C2050999&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume