4-Nonanone, 2,6,8-trimethyl-

Other names: 2,6,8-Trimethyl-4-nonanone
2,6,8-trimethylnonan-4-one
Inchi: InChI=1S/C12H24O/c1-9(2)6-11(5)8-12(13)7-10(3)4/h9-11H,6-8H2,1-5H3
InchiKey: GFWVDQCGGDBTBS-UHFFFAOYSA-N
Formula: C12H24O
SMILES: CC(C)CC(=O)CC(C)CC(C)C
Mol. weight [g/mol]: 184.32
CAS: 123-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-86.08	kJ/mol	Joback Method
hf	-419.43	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	47.89	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.674		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
tb	526.51	K	Joback Method
tc	706.79	K	Joback Method
tf	229.93	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.97	J/mol×K	526.51	Joback Method
cpg	454.06	J/mol×K	556.56	Joback Method
cpg	470.39	J/mol×K	586.60	Joback Method
cpg	485.99	J/mol×K	616.65	Joback Method
cpg	500.88	J/mol×K	646.70	Joback Method
cpg	515.07	J/mol×K	676.75	Joback Method
cpg	528.58	J/mol×K	706.79	Joback Method

dvisc	0.0159580	Pa×s	229.93	Joback Method
dvisc	0.0039939	Pa×s	279.36	Joback Method
dvisc	0.0015160	Pa×s	328.79	Joback Method
dvisc	0.0007413	Pa×s	378.22	Joback Method
dvisc	0.0004276	Pa×s	427.65	Joback Method
dvisc	0.0002765	Pa×s	477.08	Joback Method
dvisc	0.0001940	Pa×s	526.51	Joback Method

Sources

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=C123182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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