2,7-Dimethyloctan-4-one

Inchi: InChI=1S/C10H20O/c1-8(2)5-6-10(11)7-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey: FSDBXGZREACSJJ-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CC(C)CCC(=O)CC(C)C
Mol. weight [g/mol]: 156.27
CAS: 59387-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-100.48	kJ/mol	Joback Method
hf	-372.87	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	43.82	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
tb	470.00 ± 4.00	K	NIST Webbook
tc	661.30	K	Joback Method
tf	222.39	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.29	J/mol×K	481.19	Joback Method
cpg	411.92	J/mol×K	631.28	Joback Method
cpg	399.22	J/mol×K	601.26	Joback Method
cpg	385.92	J/mol×K	571.24	Joback Method
cpg	372.01	J/mol×K	541.23	Joback Method
cpg	357.47	J/mol×K	511.21	Joback Method
cpg	424.04	J/mol×K	661.30	Joback Method
dvisc	0.0002415	Pa×s	481.19	Joback Method
dvisc	0.0003333	Pa×s	438.06	Joback Method

dvisc	0.0004934	Pa×s	394.92	Joback Method
dvisc	0.0008043	Pa×s	351.79	Joback Method
dvisc	0.0015030	Pa×s	308.66	Joback Method
dvisc	0.0034410	Pa×s	265.52	Joback Method
dvisc	0.0108635	Pa×s	222.39	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=C59387927&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