2,2,4-Trimethyl-3-keto-pentanol

Inchi: InChI=1S/C8H16O2/c1-6(2)7(10)8(3,4)5-9/h6,9H,5H2,1-4H3
InchiKey: PYSAJDICZJMKGG-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(C)C(=O)C(C)(C)CO
Mol. weight [g/mol]: 144.21
CAS: 15904-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-248.86	kJ/mol	Joback Method
hf	-487.29	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.230		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	524.82	K	Joback Method
tc	706.52	K	Joback Method
tf	278.09	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.11	J/mol×K	524.82	Joback Method
cpg	324.99	J/mol×K	555.10	Joback Method
cpg	336.25	J/mol×K	585.39	Joback Method
cpg	346.92	J/mol×K	615.67	Joback Method
cpg	357.02	J/mol×K	645.95	Joback Method
cpg	366.58	J/mol×K	676.24	Joback Method
cpg	375.62	J/mol×K	706.52	Joback Method
dvisc	0.0360166	Pa×s	278.09	Joback Method
dvisc	0.0077807	Pa×s	319.21	Joback Method

dvisc	0.0023847	Pa×s	360.33	Joback Method
dvisc	0.0009312	Pa×s	401.45	Joback Method
dvisc	0.0004331	Pa×s	442.58	Joback Method
dvisc	0.0002294	Pa×s	483.70	Joback Method
dvisc	0.0001342	Pa×s	524.82	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=C15904300&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