4-Hepten-3-one, 2,6-dimethyl-

Inchi: InChI=1S/C9H16O/c1-7(2)5-6-9(10)8(3)4/h5-8H,1-4H3/b6-5+
InchiKey: FXHCGFPVKLZHCE-AATRIKPKSA-N
Formula: C9H16O
SMILES: CC(C)C=CC(=O)C(C)C
Mol. weight [g/mol]: 140.22
CAS: 56259-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-28.68	kJ/mol	Joback Method
hf	-235.01	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.424		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
ripol	1754.00		NIST Webbook
ripol	1754.00		NIST Webbook
tb	462.00 ± 4.00	K	NIST Webbook
tc	652.99	K	Joback Method
tf	206.04	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.75	J/mol×K	462.47	Joback Method
cpg	345.04	J/mol×K	621.24	Joback Method
cpg	333.65	J/mol×K	589.48	Joback Method
cpg	321.65	J/mol×K	557.73	Joback Method
cpg	309.02	J/mol×K	525.98	Joback Method
cpg	295.72	J/mol×K	494.22	Joback Method
cpg	355.84	J/mol×K	652.99	Joback Method

dvisc	0.0002146	Pa×s	462.47	Joback Method
dvisc	0.0002958	Pa×s	419.73	Joback Method
dvisc	0.0004382	Pa×s	376.99	Joback Method
dvisc	0.0007181	Pa×s	334.25	Joback Method
dvisc	0.0013599	Pa×s	291.52	Joback Method
dvisc	0.0032072	Pa×s	248.78	Joback Method
dvisc	0.0107980	Pa×s	206.04	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=C56259144&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume