4-Hepten-3-one, 2,5,6-trimethyl-

Other names: 2,5,6-Trimethyl-4-hepten-3-one
2,3,6-trimethyl-3-heptene-5-one
Inchi: InChI=1S/C10H18O/c1-7(2)9(5)6-10(11)8(3)4/h6-8H,1-5H3/b9-6+
InchiKey: BHUQHYIULGGWLZ-RMKNXTFCSA-N
Formula: C10H18O
SMILES: CC(=CC(=O)C(C)C)C(C)C
Mol. weight [g/mol]: 154.25
CAS: 16466-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-28.81	kJ/mol	Joback Method
hf	-265.44	kJ/mol	Joback Method
hfus	15.10	kJ/mol	Joback Method
hvap	43.86	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
tb	485.23	K	Joback Method
tc	677.16	K	Joback Method
tf	203.35	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.51	J/mol×K	485.23	Joback Method
cpg	340.64	J/mol×K	517.22	Joback Method
cpg	355.02	J/mol×K	549.21	Joback Method
cpg	368.68	J/mol×K	581.19	Joback Method
cpg	381.65	J/mol×K	613.18	Joback Method
cpg	393.95	J/mol×K	645.17	Joback Method
cpg	405.62	J/mol×K	677.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16466210&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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