3-Hepten-2-one, 3-ethyl-4-methyl-

Inchi: InChI=1S/C10H18O/c1-5-7-8(3)10(6-2)9(4)11/h5-7H2,1-4H3/b10-8+
InchiKey: PUHMMKUISPITSC-CSKARUKUSA-N
Formula: C10H18O
SMILES: CCCC(C)=C(CC)C(C)=O
Mol. weight [g/mol]: 154.25
CAS: 54244-90-5

Physical Properties

Property code	Value	Unit	Source
gf	-32.48	kJ/mol	Joback Method
hf	-264.67	kJ/mol	Joback Method
hfus	20.84	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	485.99	K	Joback Method
tc	673.17	K	Joback Method
tf	219.39	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.05	J/mol×K	485.99	Joback Method
cpg	339.62	J/mol×K	517.19	Joback Method
cpg	353.49	J/mol×K	548.38	Joback Method
cpg	366.69	J/mol×K	579.58	Joback Method
cpg	379.25	J/mol×K	610.78	Joback Method
cpg	391.20	J/mol×K	641.97	Joback Method
cpg	402.56	J/mol×K	673.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54244905&Units=SI

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