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

Other names: 4-Methyl-3-hepten-2-one
Inchi: InChI=1S/C8H14O/c1-4-5-7(2)6-8(3)9/h6H,4-5H2,1-3H3/b7-6+
InchiKey: URFGREAPSNSHAH-VOTSOKGWSA-N
Formula: C8H14O
SMILES: CCCC(C)=CC(C)=O
Mol. weight [g/mol]: 126.20
CAS: 22319-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-40.77	kJ/mol	Joback Method
hf	-213.60	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
ripol	1015.00		NIST Webbook
ripol	1015.00		NIST Webbook
tb	440.35	K	Joback Method
tc	627.87	K	Joback Method
tf	210.81	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.66	J/mol×K	440.35	Joback Method
cpg	252.05	J/mol×K	471.60	Joback Method
cpg	263.86	J/mol×K	502.86	Joback Method
cpg	275.09	J/mol×K	534.11	Joback Method
cpg	285.78	J/mol×K	565.36	Joback Method
cpg	295.94	J/mol×K	596.61	Joback Method

cpg	305.60	J/mol×K	627.87	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=C22319251&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume