Karahanaenone

Other names: 2,2,5-trimethyl-4-cyclohepten-1-one
Inchi: InChI=1S/C10H16O/c1-8-4-5-9(11)10(2,3)7-6-8/h6H,4-5,7H2,1-3H3
InchiKey: SKKTZNHVYFHGDC-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CCC(C)(C)C(=O)CC1
Mol. weight [g/mol]: 152.23
CAS: 19822-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-62.08	kJ/mol	Joback Method
hf	-277.72	kJ/mol	Joback Method
hfus	5.44	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1154.00		NIST Webbook
tb	524.22	K	Joback Method
tc	758.96	K	Joback Method
tf	311.72	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.26	J/mol×K	524.22	Joback Method
cpg	339.55	J/mol×K	563.34	Joback Method

cpg	356.80	J/mol×K	602.47	Joback Method
cpg	373.11	J/mol×K	641.59	Joback Method
cpg	388.56	J/mol×K	680.71	Joback Method
cpg	403.25	J/mol×K	719.83	Joback Method
cpg	417.27	J/mol×K	758.96	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=C19822674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume