Hexanal, 3-oxo-2,2,4-triethyl

Inchi: InChI=1S/C12H22O2/c1-5-10(6-2)11(14)12(7-3,8-4)9-13/h9-10H,5-8H2,1-4H3
InchiKey: STPYTSFFEKDEDC-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCC(CC)C(=O)C(C=O)(CC)CC
Mol. weight [g/mol]: 198.30
CAS: 116435-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-177.88	kJ/mol	Joback Method
hf	-503.20	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	54.09	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.997		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	572.82	K	Joback Method
tc	760.16	K	Joback Method
tf	304.35	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.30	J/mol×K	572.82	Joback Method
cpg	536.16	J/mol×K	728.93	Joback Method
cpg	523.53	J/mol×K	697.71	Joback Method
cpg	510.16	J/mol×K	666.49	Joback Method
cpg	496.02	J/mol×K	635.27	Joback Method
cpg	481.08	J/mol×K	604.04	Joback Method
cpg	548.10	J/mol×K	760.16	Joback Method
dvisc	0.0002279	Pa×s	572.82	Joback Method
dvisc	0.0003136	Pa×s	528.07	Joback Method

dvisc	0.0004577	Pa×s	483.33	Joback Method
dvisc	0.0007217	Pa×s	438.58	Joback Method
dvisc	0.0012621	Pa×s	393.84	Joback Method
dvisc	0.0025471	Pa×s	349.09	Joback Method
dvisc	0.0063191	Pa×s	304.35	Joback Method

Sources

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=C116435575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume