2,2,5-Trimethyloxepan-4-one

Inchi: InChI=1S/C9H16O2/c1-7-4-5-11-9(2,3)6-8(7)10/h7H,4-6H2,1-3H3
InchiKey: BNRJXRQVEQZRPI-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC1CCOC(C)(C)CC1=O
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-184.66	kJ/mol	Joback Method
hf	-455.73	kJ/mol	Joback Method
hfus	11.06	kJ/mol	Joback Method
hvap	43.53	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.781		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
ripol	1604.00		NIST Webbook
tb	519.48	K	Joback Method
tc	752.48	K	Joback Method
tf	309.50	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.31	J/mol×K	519.48	Joback Method
cpg	343.13	J/mol×K	558.31	Joback Method
cpg	360.92	J/mol×K	597.15	Joback Method
cpg	377.74	J/mol×K	635.98	Joback Method
cpg	393.68	J/mol×K	674.82	Joback Method
cpg	408.81	J/mol×K	713.65	Joback Method
cpg	423.22	J/mol×K	752.48	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=R228774&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume