Cyclopentanone, 2-pentyl-3-(2-oxopropyl)

Inchi: InChI=1S/C13H22O2/c1-3-4-5-8-13(10-11(2)14)9-6-7-12(13)15/h3-10H2,1-2H3
InchiKey: GTWFYHHYHLQYEV-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CCCCCC1(CC(C)=O)CCCC1=O
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-161.87	kJ/mol	Joback Method
hf	-486.21	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	54.63	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.285		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2259.00		NIST Webbook
tb	634.05	K	Joback Method
tc	845.83	K	Joback Method
tf	389.22	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.03	J/mol×K	634.05	Joback Method
cpg	529.21	J/mol×K	669.35	Joback Method
cpg	546.49	J/mol×K	704.64	Joback Method
cpg	562.97	J/mol×K	739.94	Joback Method
cpg	578.74	J/mol×K	775.23	Joback Method
cpg	593.90	J/mol×K	810.53	Joback Method

cpg	608.54	J/mol×K	845.83	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=R409626&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume