13-Hexyloxacyclotridec-10-en-2-one

Other names: (E)-13-Hexyloxacyclotridec-10-en-2-one
Inchi: InChI=1S/C18H32O2/c1-2-3-4-11-14-17-15-12-9-7-5-6-8-10-13-16-18(19)20-17/h9,12,17
InchiKey: MLZOTJKUDBBLDQ-FMIVXFBMSA-N
Formula: C18H32O2
SMILES: CCCCCCC1CC=CCCCCCCCC(=O)O1
Mol. weight [g/mol]: 280.45
CAS: 127062-51-5

Physical Properties

Property code	Value	Unit	Source
gf	-138.32	kJ/mol	Joback Method
hf	-615.57	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.559		Crippen Method
mcvol	256.760	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2071.20		NIST Webbook
rinpol	2071.20		NIST Webbook
tb	754.61	K	Joback Method
tc	986.12	K	Joback Method
tf	370.91	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.59	J/mol×K	754.61	Joback Method
cpg	834.81	J/mol×K	793.19	Joback Method
cpg	857.91	J/mol×K	831.78	Joback Method
cpg	878.85	J/mol×K	870.36	Joback Method
cpg	897.58	J/mol×K	908.95	Joback Method
cpg	914.08	J/mol×K	947.53	Joback Method

cpg	928.30	J/mol×K	986.12	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=C127062515&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