12-Methyl-oxa-cyclododecan-2-one

Other names: 11-Dodecanolide
Inchi: InChI=1S/C12H22O2/c1-11-9-7-5-3-2-4-6-8-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey: IBLSRZGJYAOPLB-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CC1CCCCCCCCCC(=O)O1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-206.70	kJ/mol	Joback Method
hf	-543.35	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	52.52	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.443		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1445.00		NIST Webbook
tb	613.90	K	Joback Method
tc	865.60	K	Joback Method
tf	306.05	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.57	J/mol×K	613.90	Joback Method
cpg	509.71	J/mol×K	655.85	Joback Method
cpg	534.12	J/mol×K	697.80	Joback Method
cpg	556.75	J/mol×K	739.75	Joback Method
cpg	577.52	J/mol×K	781.70	Joback Method
cpg	596.36	J/mol×K	823.65	Joback Method
cpg	613.19	J/mol×K	865.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U193590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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