2H-Pyran-2-one, tetrahydro-6-octyl-

Other names: 6-Octyltetrahydro-2H-pyran-2-one
«delta»-Tridecalactone
«delta»-Tridecanolide
tetrahydro-6-octyl-2H-pyran-2-one
Inchi: InChI=1S/C13H24O2/c1-2-3-4-5-6-7-9-12-10-8-11-13(14)15-12/h12H,2-11H2,1H3
InchiKey: RZZLMGATMUAJPX-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]: 212.33
CAS: 7370-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-125.68	kJ/mol	Joback Method
hf	-527.03	kJ/mol	Joback Method
hfus	28.75	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.833		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
ripol	2565.00		NIST Webbook
ripol	2565.00		NIST Webbook
tb	611.16	K	Joback Method
tc	813.34	K	Joback Method
tf	338.44	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.25	J/mol×K	611.16	Joback Method
cpg	544.15	J/mol×K	644.86	Joback Method
cpg	563.04	J/mol×K	678.55	Joback Method

cpg	580.92	J/mol×K	712.25	Joback Method
cpg	597.81	J/mol×K	745.94	Joback Method
cpg	613.70	J/mol×K	779.64	Joback Method
cpg	628.61	J/mol×K	813.34	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7370925&Units=SI

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