

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

Other names:	Octadecanoic acid, 5-hydroxy-, «delta»-lactone
Inchi:	InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-14-17-15-13-16-18(19)20-17/h17H,2-19H
InchiKey:	VVLRVPJYFLFSQG-UHFFFAOYSA-N
Formula:	C18H34O2
SMILES:	CCCCCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	282.46
CAS:	1227-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-83.58	kJ/mol	Joback Method
hf	-630.23	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.783		Crippen Method
mcvol	261.060	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
tb	725.56	K	Joback Method
tc	917.48	K	Joback Method
tf	394.79	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.34	J/mol×K	725.56	Joback Method
cpg	828.45	J/mol×K	757.55	Joback Method
cpg	848.39	J/mol×K	789.53	Joback Method
cpg	867.18	J/mol×K	821.52	Joback Method
cpg	884.84	J/mol×K	853.50	Joback Method
cpg	901.37	J/mol×K	885.49	Joback Method
cpg	916.81	J/mol×K	917.48	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=C1227516&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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