Meadowlactone

Inchi: InChI=1S/C20H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-19-17-15-18-20(21)22-19/h1
InchiKey: LLPDOHGLBDHCJZ-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: CCCCCCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]: 310.51
CAS: 110071-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-66.74	kJ/mol	Joback Method
hf	-671.51	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	69.30	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.563		Crippen Method
mcvol	289.240	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2573.10		NIST Webbook
rinpol	2573.10		NIST Webbook
tb	771.32	K	Joback Method
tc	962.25	K	Joback Method
tf	417.33	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.11	J/mol×K	771.32	Joback Method
cpg	949.46	J/mol×K	803.14	Joback Method
cpg	969.57	J/mol×K	834.96	Joback Method
cpg	988.46	J/mol×K	866.79	Joback Method
cpg	1006.17	J/mol×K	898.61	Joback Method
cpg	1022.70	J/mol×K	930.43	Joback Method
cpg	1038.08	J/mol×K	962.25	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=C110071675&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

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