«delta»-Jasmolactone

Inchi: InChI=1S/C11H18O2/c1-3-4-5-6-8-11(2)9-7-10(12)13-11/h4-5H,3,6-9H2,1-2H3/b5-4+
InchiKey: NIKDJTTZUYNCMM-SNAWJCMRSA-N
Formula: C11H18O2
SMILES: CCC=CCCC1(C)CCC(=O)O1
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-55.69	kJ/mol	Joback Method
hf	-347.13	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.828		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
ripol	1893.00		NIST Webbook
tb	565.53	K	Joback Method
tc	784.28	K	Joback Method
tf	338.24	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.21	J/mol×K	565.53	Joback Method
cpg	416.51	J/mol×K	601.99	Joback Method
cpg	432.83	J/mol×K	638.45	Joback Method
cpg	448.28	J/mol×K	674.91	Joback Method
cpg	462.98	J/mol×K	711.37	Joback Method
cpg	477.02	J/mol×K	747.83	Joback Method
cpg	490.53	J/mol×K	784.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R424556&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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