«gamma»-jasmolactone

Other names: Dec-7(Z)-en-4-olide
Inchi: InChI=1S/C10H16O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h3-4,9H,2,5-8H2,1H3/b4-3-
InchiKey: NKNGVPNCSFZRSM-ARJAWSKDSA-N
Formula: C10H16O2
SMILES: CCC=CCCC1CCC(=O)O1
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-58.62	kJ/mol	Joback Method
hf	-341.73	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.438		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2197.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2181.00		NIST Webbook
tb	542.41	K	Joback Method
tc	756.22	K	Joback Method
tf	303.07	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.95	J/mol×K	542.41	Joback Method
cpg	368.79	J/mol×K	578.04	Joback Method
cpg	384.74	J/mol×K	613.68	Joback Method
cpg	399.84	J/mol×K	649.31	Joback Method
cpg	414.09	J/mol×K	684.95	Joback Method
cpg	427.52	J/mol×K	720.58	Joback Method
cpg	440.15	J/mol×K	756.22	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=R230470&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume