marmelo lactone

Other names: 2,7-dimethyl-4-hydroxy-5(E),7-octadienoic acid lactone
trans-Marmelolactone
Inchi: InChI=1S/C10H14O2/c1-7(2)4-5-9-6-8(3)10(11)12-9/h4-5,8-9H,1,6H2,2-3H3/b5-4+
InchiKey: VOJBXZDIFIJUKD-SNAWJCMRSA-N
Formula: C10H14O2
SMILES: C=C(C)C=CC1CC(C)C(=O)O1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	12.96	kJ/mol	Joback Method
hf	-246.43	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.070		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
ripol	2127.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2139.00		NIST Webbook
ripol	2139.00		NIST Webbook
tb	534.30	K	Joback Method
tc	756.82	K	Joback Method
tf	283.11	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.62	J/mol×K	534.30	Joback Method
cpg	350.53	J/mol×K	571.39	Joback Method
cpg	366.54	J/mol×K	608.47	Joback Method
cpg	381.64	J/mol×K	645.56	Joback Method
cpg	395.86	J/mol×K	682.64	Joback Method
cpg	409.23	J/mol×K	719.73	Joback Method
cpg	421.75	J/mol×K	756.82	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=R312646&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