1,4-Dioxane-2,5-dione, 3,6-dimethyl-, (3S-cis)-

Other names:	(3S,6S)-3,6-dimethyl-1,4-dioxane-2,5-dione
	(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione
	(S,S)-lactide
	(l) 3,6-dimethyl-1,4-dioxane-2,5-dione
Inchi:	InChI=1S/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	JJTUDXZGHPGLLC-IMJSIDKUSA-N
Formula:	C6H8O4
SMILES:	CC1OC(=O)C(C)OC1=O
Mol. weight [g/mol]:	144.13
CAS:	4511-42-6

Physical Properties

Property code	Value	Unit	Source
gf	-401.04	kJ/mol	Joback Method
hf	-672.59	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Determination and Correlation of Solubility Data and Dissolution Thermodynamic Data of l-Lactide in Different Pure Solvents
hvap	46.58	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	-0.137		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	541.10	K	Joback Method
tc	782.11	K	Joback Method
tf	350.10	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.08	J/mol×K	541.10	Joback Method

cpg	259.00	J/mol×K	581.27	Joback Method
cpg	272.40	J/mol×K	621.44	Joback Method
cpg	285.18	J/mol×K	661.61	Joback Method
cpg	297.28	J/mol×K	701.78	Joback Method
cpg	308.62	J/mol×K	741.94	Joback Method
cpg	319.11	J/mol×K	782.11	Joback Method
hfust	16.94	kJ/mol	366.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4511426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase behaviour of pseudo-binary systems of pressurized ((propane + L,L-lactide)) at different methanol to L,L-lactide mole ratios:	https://www.doi.org/10.1016/j.jct.2014.06.008
High pressure phase equilibrium data for the ternary system carbon dioxide + L-lactide + ethanol:	https://www.doi.org/10.1016/j.jct.2015.02.005
Determination and Correlation of Solubility Data and Dissolution Thermodynamic Data of l-Lactide in Different Pure Solvents:	https://www.doi.org/10.1021/je301014d
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
hfust:	Enthalpy of fusion at a given temperature
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