

1,4-Dioxane-2,5-dione, 3,6-dimethyl-

Other names:	(3R,6R)-3,6-dimethyl-1,4-dioxane-2,5-dione (3R-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione 3,6-Dimethyl-1,4-dioxane-2,5-dione 3,6-Dimethyl-2,5-dioxo-1,4-dioxane D-lactide Lactide Propanoic acid, 2-hydroxy-, bimol. cyclic ester dilactide dl-Lactide p-Dioxane-2,5-dione, 3,6-dimethyl-
Inchi:	InChI=1S/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3
InchiKey:	JJTUDXZGHPGLLC-UHFFFAOYSA-N
Formula:	C6H8O4
SMILES:	CC1OC(=O)C(C)OC1=O
Mol. weight [g/mol]:	144.13
CAS:	95-96-5

Physical Properties

Property code	Value	Unit	Source
chs	-2712.50 ± 1.70	kJ/mol	NIST Webbook
gf	-401.04	kJ/mol	Joback Method
hf	-672.59	kJ/mol	Joback Method
hfs	-792.10 ± 1.70	kJ/mol	NIST Webbook
hfus	16.21	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	308.62	J/mol×K	741.94	Joback Method
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	319.11	J/mol×K	782.11	Joback Method
hfust	24.70	kJ/mol	397.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	1.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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