

methyl (R)-lactate

Other names:	Propanoic acid, 2-hydroxy-, methyl ester, (R)-
Inchi:	InChI=1S/C4H8O3/c1-3(5)4(6)7-2/h3,5H,1-2H3/t3-/m1/s1
InchiKey:	LPEKGGXMPWTOCB-GSVOUGTGSA-N
Formula:	C4H8O3
SMILES:	COC(=O)C(C)O
Mol. weight [g/mol]:	104.10
CAS:	17392-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-390.38	kJ/mol	Joback Method
hf	-528.20	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	0.27		Crippen Method
logp	-0.460		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	417.70	K	NIST Webbook
tc	636.26	K	Joback Method
tf	252.82	K	Joback Method
vc	0.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.01	J/mol×K	458.95	Joback Method
cpg	172.74	J/mol×K	488.50	Joback Method
cpg	179.25	J/mol×K	518.05	Joback Method
cpg	185.54	J/mol×K	547.60	Joback Method
cpg	191.62	J/mol×K	577.16	Joback Method
cpg	197.46	J/mol×K	606.71	Joback Method
cpg	203.08	J/mol×K	636.26	Joback Method
dvisc	0.0309613	Paxs	252.82	Joback Method

dvisc	0.0081807	Paxs	287.18	Joback Method
dvisc	0.0028726	Paxs	321.53	Joback Method
dvisc	0.0012346	Paxs	355.88	Joback Method
dvisc	0.0006157	Paxs	390.24	Joback Method
dvisc	0.0003436	Paxs	424.59	Joback Method
dvisc	0.0002093	Paxs	458.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17392835&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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