methyl (S)-(-)-lactate

Other names:	(S)-(-)-methyl lactate
	(S)-methyl 2-hydroxypropanoate
	L-methyl 2-hydroxypropanoate
	L-methyl lactate
	Propanoic acid, 2-hydroxy-, methyl ester, (S)-
	lactic acid, methyl ester, L-
	propanoic acid, 2-hydroxy-, (S)-, methyl ester
Inchi:	InChI=1S/C4H8O3/c1-3(5)4(6)7-2/h3,5H,1-2H3/t3-/m0/s1
InchiKey:	LPEKGGXMPWTOCB-VKHMYHEASA-N
Formula:	C4H8O3
SMILES:	COC(=O)C(C)O
Mol. weight [g/mol]:	104.10
CAS:	27871-49-4

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	417.00 ± 0.80	K	NIST Webbook
tb	417.70	K	NIST Webbook
tc	636.26	K	Joback Method
tf	252.82	K	Joback Method
vc	0.296	m3/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	Pa×s	252.82	Joback Method
dvisc	0.0081807	Pa×s	287.18	Joback Method
dvisc	0.0028726	Pa×s	321.53	Joback Method
dvisc	0.0012346	Pa×s	355.88	Joback Method
dvisc	0.0006157	Pa×s	390.24	Joback Method
dvisc	0.0003436	Pa×s	424.59	Joback Method
dvisc	0.0002093	Pa×s	458.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.20	K	2.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27871494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibria of N-Methylephedrine Enantiomers and Their Mixtures in Three Chiral Solvents Distinguished by Chain Length:	https://www.doi.org/10.1021/je1007839
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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