Propanoic acid, 2-hydroxy-, methyl ester, (.+/-.)-

Other names: Lactic acid, methyl ester, (.+/-.)-
Propanoic acid, 2-hydroxy-, methyl ester, (±)-
Lactic acid, methyl ester, (±)-
methyl (±)-lactate

Inchi: InChI=1S/C4H8O3/c1-3(5)4(6)7-2/h3,5H,1-2H3

InchiKey: LPEKGGXMPWTOCB-UHFFFAOYSA-N

Formula: C4H8O3

SMILES: COC(=O)C(C)O

Mol. weight [g/mol]: 104.10

CAS: 2155-30-8

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
rinpol	748.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	714.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1314.00		NIST Webbook
tb	458.95	K	Joback Method
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	197.46	J/mol×K	606.71	Joback Method
cpg	191.62	J/mol×K	577.16	Joback Method
cpg	185.54	J/mol×K	547.60	Joback Method
cpg	179.25	J/mol×K	518.05	Joback Method
cpg	172.74	J/mol×K	488.50	Joback Method
cpg	203.08	J/mol×K	636.26	Joback Method
dvisc	0.0002093	Pa×s	458.95	Joback Method
dvisc	0.0003436	Pa×s	424.59	Joback Method
dvisc	0.0006157	Pa×s	390.24	Joback Method
dvisc	0.0012346	Pa×s	355.88	Joback Method
dvisc	0.0028726	Pa×s	321.53	Joback Method
dvisc	0.0081807	Pa×s	287.18	Joback Method
dvisc	0.0309613	Pa×s	252.82	Joback Method

Sources

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=C2155308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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