Ethyl 2-(d)-hydroxy-3-methylpentanoate

Inchi: InChI=1S/C8H16O3/c1-4-6(3)7(9)8(10)11-5-2/h6-7,9H,4-5H2,1-3H3
InchiKey: TXLBCYISDOYPIH-UHFFFAOYSA-N
Formula: C8H16O3
SMILES: CCOC(=O)C(O)C(C)CC
Mol. weight [g/mol]: 160.21

Physical Properties

Property code	Value	Unit	Source
gf	-359.14	kJ/mol	Joback Method
hf	-616.04	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.956		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
ripol	1541.00		NIST Webbook
tb	550.03	K	Joback Method
tc	724.80	K	Joback Method
tf	282.90	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.04	J/mol×K	550.03	Joback Method
cpg	385.82	J/mol×K	695.67	Joback Method
cpg	376.36	J/mol×K	666.54	Joback Method
cpg	366.45	J/mol×K	637.42	Joback Method
cpg	356.10	J/mol×K	608.29	Joback Method
cpg	345.30	J/mol×K	579.16	Joback Method
cpg	394.85	J/mol×K	724.80	Joback Method

dvisc	0.0000978	Pa×s	550.03	Joback Method
dvisc	0.0001640	Pa×s	505.51	Joback Method
dvisc	0.0003039	Pa×s	460.99	Joback Method
dvisc	0.0006423	Pa×s	416.46	Joback Method
dvisc	0.0016241	Pa×s	371.94	Joback Method
dvisc	0.0052844	Pa×s	327.42	Joback Method
dvisc	0.0249265	Pa×s	282.90	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=R420554&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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