Ethyl dl-2-hydroxycaproate

Other names:	Ethyl 2-(DL)-hydroxyhexanoate
	Ethyl 2-hydroxyhexanoate
Inchi:	InChI=1S/C8H16O3/c1-3-5-6-7(9)8(10)11-4-2/h7,9H,3-6H2,1-2H3
InchiKey:	MRYSSTRVUMCKKB-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCC(O)C(=O)OCC
Mol. weight [g/mol]:	160.21
CAS:	6946-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-356.70	kJ/mol	Joback Method
hf	-610.76	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1061.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1542.00		NIST Webbook

ripol	1544.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1544.00		NIST Webbook
tb	468.20	K	NIST Webbook
tc	722.09	K	Joback Method
tf	297.90	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.69	J/mol×K	550.47	Joback Method
cpg	344.69	J/mol×K	579.07	Joback Method
cpg	355.26	J/mol×K	607.68	Joback Method
cpg	365.40	J/mol×K	636.28	Joback Method
cpg	375.11	J/mol×K	664.88	Joback Method
cpg	384.41	J/mol×K	693.49	Joback Method
cpg	393.29	J/mol×K	722.09	Joback Method
dvisc	0.0141338	Pa×s	297.90	Joback Method
dvisc	0.0037547	Pa×s	340.00	Joback Method
dvisc	0.0013358	Pa×s	382.09	Joback Method
dvisc	0.0005834	Pa×s	424.19	Joback Method
dvisc	0.0002959	Pa×s	466.28	Joback Method
dvisc	0.0001680	Pa×s	508.38	Joback Method
dvisc	0.0001040	Pa×s	550.47	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=C6946903&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