

2-Hydroxyethyl caproate

Inchi:	InChI=1S/C8H16O3/c1-2-3-4-5-8(10)11-7-6-9/h9H,2-7H2,1H3
InchiKey:	JUVBNUWZRZREEE-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCCC(=O)OCCO
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-354.26	kJ/mol	Joback Method
hf	-605.48	kJ/mol	Joback Method
hfus	23.35	kJ/mol	Joback Method
hvap	59.24	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.102		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
tb	550.91	K	Joback Method
tc	719.50	K	Joback Method
tf	312.90	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.34	J/molxK	550.91	Joback Method
cpg	383.03	J/molxK	691.40	Joback Method
cpg	373.90	J/molxK	663.30	Joback Method
cpg	364.37	J/molxK	635.20	Joback Method
cpg	354.43	J/molxK	607.11	Joback Method
cpg	344.09	J/molxK	579.01	Joback Method
cpg	391.77	J/molxK	719.50	Joback Method
dvisc	0.0001105	Paxs	550.91	Joback Method

dvisc	0.0001722	Paxs	511.24	Joback Method
dvisc	0.0002892	Paxs	471.57	Joback Method
dvisc	0.0005343	Paxs	431.90	Joback Method
dvisc	0.0011176	Paxs	392.24	Joback Method
dvisc	0.0027599	Paxs	352.57	Joback Method
dvisc	0.0085716	Paxs	312.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R540460&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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