

Pentanecarboxylic acid, 3-hydroxy-, methyl ester

Inchi:	InChI=1S/C7H12O3/c1-10-7(9)5-2-3-6(8)4-5/h5-6,8H,2-4H2,1H3
InchiKey:	ASZRODBLMORHAR-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	COC(=O)C1CCC(O)C1
Mol. weight [g/mol]:	144.17
CAS:	32811-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-333.84	kJ/mol	Joback Method
hf	-544.70	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	56.96	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.320		Crippen Method
mcvol	111.940	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	538.64	K	Joback Method
tc	732.32	K	Joback Method
tf	308.29	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.17	J/molxK	538.64	Joback Method
cpg	330.43	J/molxK	700.04	Joback Method
cpg	320.52	J/molxK	667.76	Joback Method
cpg	310.05	J/molxK	635.48	Joback Method
cpg	299.00	J/molxK	603.20	Joback Method
cpg	287.37	J/molxK	570.92	Joback Method
cpg	339.79	J/molxK	732.32	Joback Method
dvisc	0.0001871	Paxs	538.64	Joback Method
dvisc	0.0002756	Paxs	500.25	Joback Method

dvisc	0.0004332	Paxs	461.86	Joback Method
dvisc	0.0007389	Paxs	423.47	Joback Method
dvisc	0.0014021	Paxs	385.07	Joback Method
dvisc	0.0030661	Paxs	346.68	Joback Method
dvisc	0.0081473	Paxs	308.29	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=C32811760&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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