2-Pentanol, propanoate

Other names:	2-Pentyl propionate
	Propanoic acid, 1-methylbutyl ester
Inchi:	InChI=1S/C8H16O2/c1-4-6-7(3)10-8(9)5-2/h7H,4-6H2,1-3H3
InchiKey:	IPVKBEOJURLVER-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(C)OC(=O)CC
Mol. weight [g/mol]:	144.21
CAS:	54004-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	932.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	928.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1152.00		NIST Webbook
tb	458.29	K	Joback Method
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54004432&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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