

Pentanoic acid, 3-methyl-, ethyl ester

Other names:	Valeric acid, 3-methyl-, ethyl ester Ethyl «beta»-methylvalerate Ethyl 3-methylpentanoate 3-Methylpentanoic acid, ethyl ester ethyl 3-methylvalerate
Inchi:	InChI=1S/C8H16O2/c1-4-7(3)6-8(9)10-5-2/h7H,4-6H2,1-3H3
InchiKey:	TXAWGHYFBQBVNK-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCOC(=O)CC(C)CC
Mol. weight [g/mol]:	144.21
CAS:	5870-68-8

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	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	940.30		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1181.00		NIST Webbook

ripol	1168.00		NIST Webbook
tb	458.29	K	Joback Method
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/molxK	458.29	Joback Method
cpg	292.41	J/molxK	488.10	Joback Method
cpg	304.54	J/molxK	517.91	Joback Method
cpg	316.22	J/molxK	547.72	Joback Method
cpg	327.44	J/molxK	577.53	Joback Method
cpg	338.23	J/molxK	607.34	Joback Method
cpg	348.57	J/molxK	637.16	Joback Method
dvisc	0.0048246	Paxs	237.08	Joback Method
dvisc	0.0020946	Paxs	273.95	Joback Method
dvisc	0.0011084	Paxs	310.82	Joback Method
dvisc	0.0006713	Paxs	347.69	Joback Method
dvisc	0.0004476	Paxs	384.55	Joback Method
dvisc	0.0003204	Paxs	421.42	Joback Method
dvisc	0.0002420	Paxs	458.29	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=C5870688&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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