

3-Pentenoic acid, methyl ester

Other names:	Methyl 3-pentenoate Methyl ester of 3-pentenoic acid methyl pent-3-enoate
Inchi:	InChI=1S/C6H10O2/c1-3-4-5-6(7)8-2/h3-4H,5H2,1-2H3/b4-3+
InchiKey:	KJALUUCEMMPKAC-ONEGZZNKSA-N
Formula:	C6H10O2
SMILES:	CC=CCC(=O)OC
Mol. weight [g/mol]:	114.14
CAS:	818-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-154.06	kJ/mol	Joback Method
hf	-294.75	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	417.13	K	Joback Method
tc	603.73	K	Joback Method
tf	224.46	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.29	J/mol×K	417.13	Joback Method
cpg	193.78	J/mol×K	448.23	Joback Method
cpg	202.88	J/mol×K	479.33	Joback Method
cpg	211.61	J/mol×K	510.43	Joback Method
cpg	219.98	J/mol×K	541.53	Joback Method
cpg	227.98	J/mol×K	572.63	Joback Method

cpg	235.63	J/mol×K	603.73	Joback Method
dvisc	0.0027763	Pa×s	224.46	Joback Method
dvisc	0.0014062	Pa×s	256.57	Joback Method
dvisc	0.0008286	Pa×s	288.68	Joback Method
dvisc	0.0005428	Pa×s	320.80	Joback Method
dvisc	0.0003840	Pa×s	352.91	Joback Method
dvisc	0.0002879	Pa×s	385.02	Joback Method
dvisc	0.0002255	Pa×s	417.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C818586&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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