

2-Pentenoic acid, methyl ester

Other names:	Methyl 2-pentenoate Methyl pent-2-enoate
Inchi:	InChI=1S/C6H10O2/c1-3-4-5-6(7)8-2/h4-5H,3H2,1-2H3/b5-4+
InchiKey:	MBAHGFJTIVZLFB-SNAWJCMRSA-N
Formula:	C6H10O2
SMILES:	CCC=CC(=O)OC
Mol. weight [g/mol]:	114.14
CAS:	818-59-7

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
mvol	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/molxK	417.13	Joback Method
cpg	193.78	J/molxK	448.23	Joback Method
cpg	202.88	J/molxK	479.33	Joback Method
cpg	211.61	J/molxK	510.43	Joback Method
cpg	219.98	J/molxK	541.53	Joback Method
cpg	227.98	J/molxK	572.63	Joback Method
cpg	235.63	J/molxK	603.73	Joback Method

dvisc	0.0027763	Paxs	224.46	Joback Method
dvisc	0.0014062	Paxs	256.57	Joback Method
dvisc	0.0008286	Paxs	288.68	Joback Method
dvisc	0.0005428	Paxs	320.80	Joback Method
dvisc	0.0003840	Paxs	352.91	Joback Method
dvisc	0.0002879	Paxs	385.02	Joback Method
dvisc	0.0002255	Paxs	417.13	Joback Method

Sources

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=C818597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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