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: CC/C=C/C(=O)OC
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
af	0.3705		Cheméo Relay (1.0)
hf	-370.91	kJ/mol	Cheméo Relay (1.0)
hfus	14.28	kJ/mol	Joback Method
hvap	43.11	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-1.79		Cheméo Relay (1.0)
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	390.93	K	Cheméo Relay (1.0)
tc	593.20	K	Cheméo Relay (1.0)
tf	225.41	K	Cheméo Relay (1.0)
vc	0.351	m3/kmol	Cheméo Relay (1.0)

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=C818597&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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