5-Methyl-(E)-2-hepten-4-one

Other names: (2E)-5-Methyl-2-hepten-4-one
(E)-5-methyl-2-hepten-4-one
Filbertone, (.+/-.)-
(E)-5-methyl-2-hepten-4-one (Filbertone)
2-Hepten-4-one, 5-methyl-, (2E)-
Filbertone 5-Methyl-2-Hepten-4-one
Inchi: InChI=1S/C8H14O/c1-4-6-8(9)7(3)5-2/h4,6-7H,5H2,1-3H3/b6-4+
InchiKey: ARJWAURHQDJJAC-GQCTYLIASA-N
Formula: C8H14O
SMILES: CC=CC(=O)C(C)CC
Mol. weight [g/mol]: 126.20
CAS: 102322-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-34.66	kJ/mol	Joback Method
hf	-209.09	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	39.72	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	970.00		NIST Webbook
rinpol	972.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1287.00		NIST Webbook
tb	440.03	K	Joback Method
tc	628.20	K	Joback Method
tf	209.77	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.81	J/mol×K	440.03	Joback Method
cpg	252.37	J/mol×K	471.39	Joback Method
cpg	264.33	J/mol×K	502.75	Joback Method
cpg	275.70	J/mol×K	534.12	Joback Method
cpg	286.51	J/mol×K	565.48	Joback Method
cpg	296.79	J/mol×K	596.84	Joback Method
cpg	306.55	J/mol×K	628.20	Joback Method
dvisc	0.0063735	Pa×s	209.77	Joback Method
dvisc	0.0024014	Pa×s	248.15	Joback Method
dvisc	0.0011752	Pa×s	286.52	Joback Method
dvisc	0.0006809	Pa×s	324.90	Joback Method
dvisc	0.0004427	Pa×s	363.28	Joback Method
dvisc	0.0003125	Pa×s	401.65	Joback Method
dvisc	0.0002344	Pa×s	440.03	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=C102322838&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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