PENTYL ACETOACETATE

Other names: Acetoacetic acid, n-amyl ester
Pentyl 3-oxobutanoate
Inchi: InChI=1S/C9H16O3/c1-3-4-5-6-12-9(11)7-8(2)10/h3-7H2,1-2H3
InchiKey: IDZAUPYMMSSVHP-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CCCCCOC(=O)CC(C)=O
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
af	0.6062		Cheméo Relay (1.0)
hf	-663.63	kJ/mol	Cheméo Relay (1.0)
hfus	23.45	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.699		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	493.99	K	Cheméo Relay (1.0)
tc	677.43	K	Cheméo Relay (1.0)
tf	243.17	K	Cheméo Relay (1.0)
vc	0.548	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.51	J/mol×K	535.48	Joback Method
cpg	356.03	J/mol×K	565.94	Joback Method
cpg	368.04	J/mol×K	596.41	Joback Method
cpg	379.53	J/mol×K	626.87	Joback Method
cpg	390.51	J/mol×K	657.34	Joback Method
cpg	400.99	J/mol×K	687.80	Joback Method
cpg	410.97	J/mol×K	718.27	Joback Method

dvisc	0.0026992	Pa×s	313.28	Joback Method
dvisc	0.0014842	Pa×s	350.31	Joback Method
dvisc	0.0009150	Pa×s	387.35	Joback Method
dvisc	0.0006138	Pa×s	424.38	Joback Method
dvisc	0.0004390	Pa×s	461.41	Joback Method
dvisc	0.0003300	Pa×s	498.45	Joback Method
dvisc	0.0002580	Pa×s	535.48	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6624846&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

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