

Pentyl acetoacetate

Other names:	Pentyl 3-oxobutanoate Acetoacetic acid, n-amyl ester
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
CAS:	6624-84-6

Physical Properties

Property code	Value	Unit	Source
gf	-337.94	kJ/mol	Joback Method
hf	-586.47	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.699		Crippen Method
mvol	146.680	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	495.00	K	NIST Webbook
tc	718.27	K	Joback Method
tf	313.28	K	Joback Method
vc	0.570	m ³ /kmol	Joback Method

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	Paxs	313.28	Joback Method
dvisc	0.0014842	Paxs	350.31	Joback Method
dvisc	0.0009150	Paxs	387.35	Joback Method
dvisc	0.0006138	Paxs	424.38	Joback Method
dvisc	0.0004390	Paxs	461.41	Joback Method
dvisc	0.0003300	Paxs	498.45	Joback Method
dvisc	0.0002580	Paxs	535.48	Joback Method

Sources

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

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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