

3,4-Pentadienal

Inchi:	InChI=1S/C5H6O/c1-2-3-4-5-6/h3,5H,1,4H2
InchiKey:	ZAHREXMSTLJYPJ-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	C=C=CCC=O
Mol. weight [g/mol]:	82.10
CAS:	4009-55-6

Physical Properties

Property code	Value	Unit	Source
gf	107.82	kJ/mol	Joback Method
hf	56.10	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	33.21	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.916		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	362.41	K	Joback Method
tc	551.04	K	Joback Method
tf	192.86	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.27	J/molxK	362.41	Joback Method
cpg	129.59	J/molxK	393.85	Joback Method
cpg	135.70	J/molxK	425.29	Joback Method
cpg	141.60	J/molxK	456.72	Joback Method
cpg	147.29	J/molxK	488.16	Joback Method
cpg	152.76	J/molxK	519.60	Joback Method
cpg	158.03	J/molxK	551.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4009556&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	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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