

2,4-pentadienal

Inchi:	InChI=1S/C5H6O/c1-2-3-4-5-6/h2-5H,1H2/b4-3+
InchiKey:	PPXGQLMPUIVFRE-ONEGZZNKSA-N
Formula:	C5H6O
SMILES:	C=CC=CC=O
Mol. weight [g/mol]:	82.10
CAS:	764-40-9

Physical Properties

Property code	Value	Unit	Source
gf	59.76	kJ/mol	Joback Method
hf	10.54	kJ/mol	Joback Method
hfus	9.92	kJ/mol	Joback Method
hvap	32.73	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.927		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
ripol	1197.00		NIST Webbook
ripol	1197.00		NIST Webbook
tb	363.30	K	Joback Method
tc	549.54	K	Joback Method
tf	181.27	K	Joback Method
vc	0.293	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.66	J/mol×K	363.30	Joback Method
cpg	124.03	J/mol×K	394.34	Joback Method
cpg	130.99	J/mol×K	425.38	Joback Method
cpg	137.55	J/mol×K	456.42	Joback Method
cpg	143.73	J/mol×K	487.46	Joback Method
cpg	149.55	J/mol×K	518.50	Joback Method
cpg	155.03	J/mol×K	549.54	Joback Method

dvisc	0.0027667	Paxs	181.27	Joback Method
dvisc	0.0013740	Paxs	211.61	Joback Method
dvisc	0.0008133	Paxs	241.95	Joback Method
dvisc	0.0005411	Paxs	272.28	Joback Method
dvisc	0.0003906	Paxs	302.62	Joback Method
dvisc	0.0002993	Paxs	332.96	Joback Method
dvisc	0.0002397	Paxs	363.30	Joback Method

Sources

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=C764409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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