

4-Penten-2-one, 4-methyl-

Other names:	2-Methyl-1-penten-4-one 2-Methylene-4-pentanal 4-Methyl-4-penten-2-one <chem>CH3C(O)CH2C(CH3)=CH2</chem> Isomesityl oxide Isopropenyl acetone
Inchi:	InChI=1S/C6H10O/c1-5(2)4-6(3)7/h1,4H2,2-3H3
InchiKey:	VADUDTKCGJKNDY-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	<chem>C=C(C)CC(C)=O</chem>
Mol. weight [g/mol]:	98.14
CAS:	3744-02-3

Physical Properties

Property code	Value	Unit	Source
gf	-49.99	kJ/mol	Joback Method
hf	-164.11	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	41.90	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	790.00		NIST Webbook
ripol	1110.00		NIST Webbook
tb	387.11	K	Joback Method
tc	572.11	K	Joback Method
tf	200.55 ± 0.20	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/mol×K	387.11	Joback Method

cpg	172.98	J/mol×K	417.94	Joback Method
cpg	182.16	J/mol×K	448.78	Joback Method
cpg	190.92	J/mol×K	479.61	Joback Method
cpg	199.29	J/mol×K	510.45	Joback Method
cpg	207.28	J/mol×K	541.28	Joback Method
cpg	214.90	J/mol×K	572.11	Joback Method
hvapt	36.90	kJ/mol	425.00	NIST Webbook
hvapt	41.10	kJ/mol	352.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34033e+01
Coeff. B	-3.13505e+03
Coeff. C	-5.49620e+01
Temperature range (K), min.	293.99
Temperature range (K), max.	442.40

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C3744023&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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

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