

3-Penten-1-yne, 3-methyl-

Other names:	3-Methyl-3-penten-1-yne 3-methylpent-3-en-1-yne
Inchi:	InChI=1S/C6H8/c1-4-6(3)5-2/h1,5H,2-3H3/b6-5+
InchiKey:	GRGVQLWQXHFRHO-AATRIKPKSA-N
Formula:	C6H8
SMILES:	C#CC(C)=CC
Mol. weight [g/mol]:	80.13
CAS:	1574-33-0

Physical Properties

Property code	Value	Unit	Source
gf	294.38	kJ/mol	Joback Method
hf	232.16	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	28.85	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.586		Crippen Method
mvol	82.500	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	342.00 ± 2.00	K	NIST Webbook
tc	520.04	K	Joback Method
tf	185.31	K	Joback Method
vc	0.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.23	J/mol×K	330.84	Joback Method
cpg	134.04	J/mol×K	362.37	Joback Method
cpg	142.36	J/mol×K	393.91	Joback Method
cpg	150.21	J/mol×K	425.44	Joback Method
cpg	157.63	J/mol×K	456.97	Joback Method
cpg	164.62	J/mol×K	488.51	Joback Method
cpg	171.23	J/mol×K	520.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49869e+01
Coeff. B	-3.17722e+03
Coeff. C	-3.55730e+01
Temperature range (K), min.	251.72
Temperature range (K), max.	363.95

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1574330&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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