

2-Pentene, 3-methyl-

Other names:	3-Methyl-2-pentene 3-Methyl-2-pentene,c&t 3-methylpent-2-ene CH3CH=C(CH3)C2H5
Inchi:	InChI=1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3
InchiKey:	BEQGRRJLJLVQAQ-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CC=C(C)CC
Mol. weight [g/mol]:	84.16
CAS:	922-61-2

Physical Properties

Property code	Value	Unit	Source
affp	812.90	kJ/mol	NIST Webbook
basg	784.00	kJ/mol	NIST Webbook
gf	71.31	kJ/mol	Joback Method
hf	-59.74	kJ/mol	Joback Method
hfus	10.19	kJ/mol	Joback Method
hvap	28.99	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	617.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	610.00		NIST Webbook
tb	340.72	K	Joback Method
tc	516.68	K	Joback Method
tf	138.34	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.07	J/mol×K	340.72	Joback Method
cpg	155.60	J/mol×K	370.05	Joback Method
cpg	165.66	J/mol×K	399.37	Joback Method
cpg	175.29	J/mol×K	428.70	Joback Method
cpg	184.49	J/mol×K	458.03	Joback Method
cpg	193.27	J/mol×K	487.36	Joback Method
cpg	201.67	J/mol×K	516.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48533e+01
Coeff. B	-3.12257e+03
Coeff. C	-3.59620e+01
Temperature range (K), min.	250.34
Temperature range (K), max.	363.21

Sources

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=C922612&Units=SI
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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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