

2-Pentene, 2,3-dimethyl-

Other names:	2,3-DIMETHYL-2-PENTENE C2H5C(CH3)=C(CH3)2 ETHYLTRIMETHYLETHYLENE
Inchi:	InChI=1S/C7H14/c1-5-7(4)6(2)3/h5H2,1-4H3
InchiKey:	WFHALSLYRWWUGH-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCC(C)=C(C)C
Mol. weight [g/mol]:	98.19
CAS:	10574-37-5

Physical Properties

Property code	Value	Unit	Source
gf	71.18	kJ/mol	Joback Method
hf	-90.17	kJ/mol	Joback Method
hfus	11.47	kJ/mol	Joback Method
hvap	35.60	kJ/mol	NIST Webbook
ie	8.21 ± 0.01	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	712.00		NIST Webbook
rinpol	712.80		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	712.20		NIST Webbook
rinpol	703.30		NIST Webbook
rinpol	704.40		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	703.10		NIST Webbook
rinpol	703.50		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	703.00		NIST Webbook

rinpol	706.20		NIST Webbook
rinpol	708.70		NIST Webbook
rinpol	708.70		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	715.50		NIST Webbook
rinpol	703.40		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	712.80		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	702.10		NIST Webbook
tb	366.65 ± 5.00	K	NIST Webbook
tb	367.15 ± 3.00	K	NIST Webbook
tb	364.00 ± 5.00	K	NIST Webbook
tb	370.70	K	NIST Webbook
tb	370.55 ± 0.50	K	NIST Webbook
tb	370.53 ± 0.20	K	NIST Webbook
tb	370.65 ± 1.00	K	NIST Webbook
tb	370.61 ± 0.30	K	NIST Webbook
tb	370.15 ± 1.00	K	NIST Webbook
tb	370.49 ± 0.60	K	NIST Webbook
tb	370.58 ± 0.30	K	NIST Webbook
tb	370.49 ± 0.30	K	NIST Webbook

tb	370.49 ± 0.40	K	NIST Webbook
tb	97.65 ± 0.50	K	NIST Webbook
tb	368.25 ± 0.70	K	NIST Webbook
tb	365.65 ± 4.00	K	NIST Webbook
tb	365.65 ± 4.00	K	NIST Webbook
tb	366.15 ± 4.00	K	NIST Webbook
tb	967.15 ± 2.00	K	NIST Webbook
tb	366.65 ± 3.00	K	NIST Webbook
tb	364.65 ± 4.00	K	NIST Webbook
tc	542.91	K	Joback Method
tf	135.65	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.35	J/mol×K	363.48	Joback Method
cpg	192.44	J/mol×K	393.38	Joback Method
cpg	204.00	J/mol×K	423.29	Joback Method
cpg	215.05	J/mol×K	453.19	Joback Method
cpg	225.59	J/mol×K	483.10	Joback Method
cpg	235.66	J/mol×K	513.00	Joback Method
cpg	245.27	J/mol×K	542.91	Joback Method
hvapt	34.20	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41363e+01
Coeff. B	-3.00625e+03
Coeff. C	-5.21500e+01
Temperature range (K), min.	269.23
Temperature range (K), max.	392.81

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10574375&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=241

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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