1-Pentene, 2,3-dimethyl-

Other names: 2,3-Dimethyl-1-pentene
2,3-dimethylpent-1-ene
Inchi: InChI=1S/C7H14/c1-5-7(4)6(2)3/h7H,2,5H2,1,3-4H3
InchiKey: LIMAEKMEXJTSNI-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=C(C)C(C)CC
Mol. weight [g/mol]: 98.19
CAS: 3404-72-6

Physical Properties

Property code	Value	Unit	Source
gf	84.91	kJ/mol	Joback Method
hf	-77.45	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	30.20	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	658.00		NIST Webbook
rinpol	648.30		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	656.90		NIST Webbook
rinpol	658.50		NIST Webbook
rinpol	650.60		NIST Webbook
rinpol	652.20		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	650.00		NIST Webbook

rinpol	657.60		NIST Webbook
rinpol	652.00		NIST Webbook
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rinpol	654.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	649.00		NIST Webbook
tb	355.68	K	Joback Method
tc	533.60	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	137.93	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.34	J/mol×K	355.68	Joback Method
cpg	192.16	J/mol×K	384.75	Joback Method
cpg	203.51	J/mol×K	413.82	Joback Method
cpg	214.40	J/mol×K	442.89	Joback Method
cpg	224.84	J/mol×K	471.96	Joback Method
cpg	234.84	J/mol×K	501.04	Joback Method
cpg	244.42	J/mol×K	530.11	Joback Method
hvapt	33.40	kJ/mol	346.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38793e+01
Coeff. B	-2.82729e+03
Coeff. C	-5.21380e+01
Temperature range (K), min.	260.15
Temperature range (K), max.	382.13

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=235
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404726&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume