2-Pentene, 3,4-dimethyl-

Other names: 3,4-Dimethyl-2-pentene
3,4-dimethylpent-2-ene
Inchi: InChI=1S/C7H14/c1-5-7(4)6(2)3/h5-6H,1-4H3
InchiKey: PPBWEVVDSRKEIK-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC=C(C)C(C)C
Mol. weight [g/mol]: 98.19
CAS: 24910-63-2

Physical Properties

Property code	Value	Unit	Source
gf	77.29	kJ/mol	Joback Method
hf	-85.66	kJ/mol	Joback Method
hfus	9.25	kJ/mol	Joback Method
hvap	30.83	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	719.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	138.80		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	671.00		NIST Webbook
tb	359.45 ± 0.50	K	NIST Webbook
tb	360.15 ± 3.00	K	NIST Webbook
tb	359.45 ± 2.00	K	NIST Webbook
tc	543.24	K	Joback Method
tf	134.61	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.18	J/mol×K	363.16	Joback Method
cpg	192.45	J/mol×K	393.17	Joback Method
cpg	204.18	J/mol×K	423.19	Joback Method
cpg	215.38	J/mol×K	453.20	Joback Method
cpg	226.07	J/mol×K	483.22	Joback Method
cpg	236.27	J/mol×K	513.23	Joback Method
cpg	246.01	J/mol×K	543.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50466e+01
Coeff. B	-3.31617e+03
Coeff. C	-4.14520e+01
Temperature range (K), min.	266.14
Temperature range (K), max.	382.09

Sources

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=C24910632&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume