CH3CH=C(CH3)C2H5

Other names: 3-Methyl-2-pentene
3-Methyl-2-pentene,c&t
3-methylpent-2-ene
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
af	0.2317		Cheméo Relay (1.0)
affp	812.90	kJ/mol	NIST Webbook
basg	784.00	kJ/mol	NIST Webbook
gf	71.31	kJ/mol	Joback Method
hf	-78.95	kJ/mol	Cheméo Relay (1.0)
hfus	10.19	kJ/mol	Joback Method
hvap	29.67	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	589.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	610.00		NIST Webbook
tb	341.00 ± 0.60	K	NIST Webbook
tb	341.00 ± 4.00	K	NIST Webbook
tb	340.65 ± 4.00	K	NIST Webbook
tb	309.15 ± 0.50	K	NIST Webbook
tb	342.00 ± 3.00	K	NIST Webbook
tb	343.00 ± 6.00	K	NIST Webbook
tb	342.20	K	NIST Webbook

tc	500.72	K	Cheméo Relay (1.0)
tf	144.43	K	Cheméo Relay (1.0)
vc	0.337	m3/kmol	Cheméo Relay (1.0)

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(Pvp) = 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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C922612&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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