1-Butene, 2-ethyl-3-methyl-

Other names: 2-ETHYL-3-METHYL-1-BUTENE
2-ETHYL-3-METHYLBUT-1-ENE
3-Methyl-2-ethyl-1-butene
Inchi: InChI=1S/C7H14/c1-5-7(4)6(2)3/h6H,4-5H2,1-3H3
InchiKey: ADHCYQWFCLQBFG-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=C(CC)C(C)C
Mol. weight [g/mol]: 98.19
CAS: 7357-93-9

Physical Properties

Property code	Value	Unit	Source
chl	-4641.30 ± 1.30	kJ/mol	NIST Webbook
gf	84.91	kJ/mol	Joback Method
hf	-77.45	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
hvap	34.40	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	661.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	662.70		NIST Webbook
rinpol	667.60		NIST Webbook
rinpol	658.60		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	655.00		NIST Webbook

rinpol	652.00		NIST Webbook
rinpol	658.60		NIST Webbook
rinpol	665.80		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	658.30		NIST Webbook
rinpol	665.80		NIST Webbook
tb	355.68	K	Joback Method
tc	530.11	K	Joback Method
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	33.80	kJ/mol	342.00	NIST Webbook
hvapt	34.40	kJ/mol	325.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37547e+01
Coeff. B	-2.82559e+03
Coeff. C	-5.17310e+01
Temperature range (K), min.	261.55
Temperature range (K), max.	386.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.13750e+01
Coeff. B	-7.08570e+03
Coeff. C	-1.16232e+01
Coeff. D	1.04615e-05
Temperature range (K), min.	290.15
Temperature range (K), max.	359.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol247.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7357939&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=247
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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