1-Pentene, 3-ethyl-2-methyl-

Other names: 2-Methyl-3-ethyl-1-pentene
3-ETHYL-2-METHYL-1-PENTENE
3-Ethyl-2-methylpent-1-ene
Inchi: InChI=1S/C8H16/c1-5-8(6-2)7(3)4/h8H,3,5-6H2,1-2,4H3
InchiKey: HPHHYSWOBXEIRG-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C)C(CC)CC
Mol. weight [g/mol]: 112.21
CAS: 19780-66-6

Physical Properties

Property code	Value	Unit	Source
chl	-5296.99 ± 0.75	kJ/mol	NIST Webbook
gf	93.33	kJ/mol	Joback Method
hf	-98.09	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	37.70	kJ/mol	NIST Webbook
hvap	37.50	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	737.00		NIST Webbook
rinpol	754.30		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	754.30		NIST Webbook
rinpol	746.70		NIST Webbook
rinpol	735.19		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	735.00		NIST Webbook
tb	382.41 ± 0.20	K	NIST Webbook
tb	382.42 ± 0.20	K	NIST Webbook
tb	382.70	K	NIST Webbook

tc	552.61	K	Joback Method
tf	160.20 ± 0.04	K	NIST Webbook
tf	160.20 ± 0.06	K	NIST Webbook
tf	160.25 ± 0.02	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.59	J/mol×K	378.56	Joback Method
cpg	230.69	J/mol×K	407.57	Joback Method
cpg	243.26	J/mol×K	436.58	Joback Method
cpg	255.31	J/mol×K	465.59	Joback Method
cpg	266.87	J/mol×K	494.59	Joback Method
cpg	277.94	J/mol×K	523.60	Joback Method
cpg	288.55	J/mol×K	552.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42426e+01
Coeff. B	-3.26001e+03
Coeff. C	-4.39730e+01
Temperature range (K), min.	277.58
Temperature range (K), max.	408.99

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.70103e+01
Coeff. B	-7.29871e+03
Coeff. C	-1.08574e+01
Coeff. D	8.59909e-06
Temperature range (K), min.	308.15
Temperature range (K), max.	382.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=324
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/files/research/kdb/mol/mol324.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780666&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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