

1-Pentene, 3-ethyl-4-methyl-

Other names:	3-ETHYL-4-METHYL-1-PENTENE 3-Ethyl-4-methylpent-1-ene 4-METHYL-3-ETHYL-1-PENTENE
Inchi:	InChI=1S/C8H16/c1-5-8(6-2)7(3)4/h5,7-8H,1,6H2,2-4H3
InchiKey:	DTNALCAUPPLROB-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=CC(CC)C(C)C
Mol. weight [g/mol]:	112.21
CAS:	61847-80-1

Physical Properties

Property code	Value	Unit	Source
gf	99.44	kJ/mol	Joback Method
hf	-93.58	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	731.00		NIST Webbook
rinpol	720.80		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	731.80		NIST Webbook
rinpol	731.80		NIST Webbook
tb	380.70 ± 1.00	K	NIST Webbook
tc	552.91	K	Joback Method
tf	148.16	K	Joback Method
vc	0.453	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	217.47	J/molxK	378.24	Joback Method
cpg	230.74	J/molxK	407.35	Joback Method
cpg	243.47	J/molxK	436.46	Joback Method
cpg	255.68	J/molxK	465.57	Joback Method
cpg	267.38	J/molxK	494.69	Joback Method
cpg	278.59	J/molxK	523.80	Joback Method
cpg	289.32	J/molxK	552.91	Joback Method
dvisc	0.0184203	Paxs	148.16	Joback Method
dvisc	0.0041486	Paxs	186.51	Joback Method
dvisc	0.0015535	Paxs	224.85	Joback Method
dvisc	0.0007745	Paxs	263.20	Joback Method
dvisc	0.0004609	Paxs	301.55	Joback Method
dvisc	0.0003084	Paxs	339.89	Joback Method
dvisc	0.0002238	Paxs	378.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39091e+01
Coeff. B	-2.99688e+03
Coeff. C	-5.81340e+01
Temperature range (K), min.	278.15
Temperature range (K), max.	406.71

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=326
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61847801&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
dvisc:	Dynamic viscosity
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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