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

Other names: 3-Ethyl-3-methyl-1-pentene
3-Ethyl-3-methylpent-1-ene
Inchi: InChI=1S/C8H16/c1-5-8(4,6-2)7-3/h5H,1,6-7H2,2-4H3
InchiKey: PHHHEKOJKDYRIN-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CC(C)(CC)CC
Mol. weight [g/mol]: 112.21
CAS: 6196-60-7

Physical Properties

Property code	Value	Unit	Source
gf	107.16	kJ/mol	Joback Method
hf	-91.77	kJ/mol	Joback Method
hfus	7.78	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	744.30		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	740.10		NIST Webbook
rinpol	744.30		NIST Webbook
tb	383.70 ± 1.00	K	NIST Webbook
tc	553.76	K	Joback Method
tf	180.58	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/mol×K	375.89	Joback Method
cpg	232.71	J/mol×K	405.54	Joback Method
cpg	246.11	J/mol×K	435.18	Joback Method

cpg	258.84	J/mol×K	464.83	Joback Method
cpg	270.93	J/mol×K	494.47	Joback Method
cpg	282.41	J/mol×K	524.12	Joback Method
cpg	293.30	J/mol×K	553.76	Joback Method
dvisc	0.0095731	Pa×s	180.58	Joback Method
dvisc	0.0033567	Pa×s	213.13	Joback Method
dvisc	0.0015537	Pa×s	245.68	Joback Method
dvisc	0.0008612	Pa×s	278.24	Joback Method
dvisc	0.0005402	Pa×s	310.79	Joback Method
dvisc	0.0003702	Pa×s	343.34	Joback Method
dvisc	0.0002708	Pa×s	375.89	Joback Method

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/mol325.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6196607&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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