1-Pentene, 2-(1-methylethyl)

Other names: 2-Isopropyl-1-pentene
2-Isopropylpent-1-ene
Inchi: InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h7H,4-6H2,1-3H3
InchiKey: QOUCFWFZPKWYRE-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(CCC)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 16746-02-4

Physical Properties

Property code	Value	Unit	Source
gf	93.33	kJ/mol	Joback Method
hf	-98.09	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	32.42	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	753.70		NIST Webbook
rinpol	744.40		NIST Webbook
rinpol	748.50		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	747.00		NIST Webbook
tb	378.56	K	Joback Method
tc	552.61	K	Joback Method
tf	149.20	K	Joback Method
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	1.34742e+01
Coeff. B	-3.03275e+03
Coeff. C	-5.08960e+01
Temperature range (K), min.	280.88
Temperature range (K), max.	422.43

Sources

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/mol321.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16746024&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

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