1-Pentene, 4-methyl-2-propyl

Inchi: InChI=1S/C9H18/c1-5-6-9(4)7-8(2)3/h8H,4-7H2,1-3H3
InchiKey: LKZBMUCWYPLUND-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(CCC)CC(C)C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	101.75	kJ/mol	Joback Method
hf	-118.73	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	34.65	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	825.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
tb	401.44	K	Joback Method
tc	574.80	K	Joback Method
tf	160.47	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.19	J/mol×K	401.44	Joback Method
cpg	271.44	J/mol×K	430.33	Joback Method
cpg	285.11	J/mol×K	459.23	Joback Method
cpg	298.22	J/mol×K	488.12	Joback Method
cpg	310.78	J/mol×K	517.01	Joback Method
cpg	322.81	J/mol×K	545.91	Joback Method

cpg	334.34	J/mol×K	574.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R3591&Units=SI
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

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