2-propyl-1-hexene

Inchi: InChI=1S/C9H18/c1-4-6-8-9(3)7-5-2/h3-8H2,1-2H3
InchiKey: BWGGEKJMCRHXKX-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(CCC)CCCC
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	104.19	kJ/mol	Joback Method
hf	-113.45	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
tb	401.88	K	Joback Method
tc	571.36	K	Joback Method
tf	175.47	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.27	J/mol×K	401.88	Joback Method
cpg	271.11	J/mol×K	430.13	Joback Method
cpg	284.40	J/mol×K	458.37	Joback Method
cpg	297.17	J/mol×K	486.62	Joback Method
cpg	309.42	J/mol×K	514.87	Joback Method
cpg	321.16	J/mol×K	543.11	Joback Method
cpg	332.43	J/mol×K	571.36	Joback Method

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R141281&Units=SI

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