1-Heptyne, 6-methyl

Inchi: InChI=1S/C8H14/c1-4-5-6-7-8(2)3/h1,8H,5-7H2,2-3H3
InchiKey: CODOVMCZKJILBE-UHFFFAOYSA-N
Formula: C8H14
SMILES: C#CCCCC(C)C
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
gf	237.11	kJ/mol	Joback Method
hf	78.17	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	32.87	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
tb	372.12	K	Joback Method
tc	551.24	K	Joback Method
tf	211.89	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.61	J/mol×K	372.12	Joback Method
cpg	219.67	J/mol×K	401.97	Joback Method
cpg	231.21	J/mol×K	431.83	Joback Method
cpg	242.26	J/mol×K	461.68	Joback Method
cpg	252.83	J/mol×K	491.54	Joback Method
cpg	262.93	J/mol×K	521.39	Joback Method
cpg	272.59	J/mol×K	551.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66465&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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