1-Hexyl radical

Inchi: InChI=1S/C6H13/c1-3-5-6-4-2/h1,3-6H2,2H3
InchiKey: PQGAHNJECSVDEI-UHFFFAOYSA-N
Formula: C6H13
SMILES: [CH2]CCCCC
Mol. weight [g/mol]: 85.17
CAS: 2679-29-0

Physical Properties

Property code	Value	Unit	Source
gf	52.02	kJ/mol	Joback Method
hf	-111.36	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	28.80	kJ/mol	Joback Method
ie	7.92 ± 0.06	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	2.401		Crippen Method
mcvol	93.250	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	335.98	K	Joback Method
tc	496.27	K	Joback Method
tf	173.75	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.29	J/mol×K	335.98	Joback Method
cpg	163.51	J/mol×K	362.70	Joback Method
cpg	173.26	J/mol×K	389.41	Joback Method
cpg	182.56	J/mol×K	416.13	Joback Method
cpg	191.44	J/mol×K	442.84	Joback Method
cpg	199.91	J/mol×K	469.56	Joback Method
cpg	207.99	J/mol×K	496.27	Joback Method
dvisc	0.0008702	Pa×s	173.75	Joback Method

dvisc	0.0006278	Pa×s	200.79	Joback Method
dvisc	0.0004894	Pa×s	227.83	Joback Method
dvisc	0.0004023	Pa×s	254.87	Joback Method
dvisc	0.0003433	Pa×s	281.90	Joback Method
dvisc	0.0003012	Pa×s	308.94	Joback Method
dvisc	0.0002699	Pa×s	335.98	Joback Method

Sources

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=C2679290&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume