2-Hexyl radical

Inchi: InChI=1S/C6H13/c1-3-5-6-4-2/h3H,4-6H2,1-2H3
InchiKey: UKTLNAIDPLDTPZ-UHFFFAOYSA-N
Formula: C6H13
SMILES: C[CH]CCCC
Mol. weight [g/mol]: 85.17
CAS: 2493-44-9

Physical Properties

Property code	Value	Unit	Source
gf	49.58	kJ/mol	Joback Method
hf	-116.64	kJ/mol	Joback Method
hfus	9.46	kJ/mol	Joback Method
hvap	28.41	kJ/mol	Joback Method
ie	7.38	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	2.401		Crippen Method
mcvol	93.250	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	335.54	K	Joback Method
tc	499.69	K	Joback Method
tf	158.75	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.04	J/mol×K	335.54	Joback Method
cpg	163.60	J/mol×K	362.90	Joback Method
cpg	173.67	J/mol×K	390.26	Joback Method
cpg	183.26	J/mol×K	417.62	Joback Method
cpg	192.40	J/mol×K	444.98	Joback Method
cpg	201.11	J/mol×K	472.33	Joback Method
cpg	209.41	J/mol×K	499.69	Joback Method
dvisc	0.0012145	Pa×s	158.75	Joback Method

dvisc	0.0007723	Pa×s	188.22	Joback Method
dvisc	0.0005551	Pa×s	217.68	Joback Method
dvisc	0.0004317	Pa×s	247.14	Joback Method
dvisc	0.0003542	Pa×s	276.61	Joback Method
dvisc	0.0003019	Pa×s	306.07	Joback Method
dvisc	0.0002646	Pa×s	335.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2493449&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
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

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