

Hexadecane, 4-hexyl

Inchi:	InChI=1S/C22H46/c1-4-7-9-11-12-13-14-15-16-18-21-22(19-6-3)20-17-10-8-5-2/h22H,4-
InchiKey:	BUIUBTKDFHPLNN-UHFFFAOYSA-N
Formula:	C22H46
SMILES:	CCCCCCCCCCCC(CCC)CCCCC
Mol. weight [g/mol]:	310.60

Physical Properties

Property code	Value	Unit	Source
gf	131.92	kJ/mol	Joback Method
hf	-502.69	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinsol	2095.00		NIST Webbook
tb	702.32	K	Joback Method
tc	867.26	K	Joback Method
tf	322.70	K	Joback Method
vc	1.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.39	J/molxK	702.32	Joback Method
cpg	984.38	J/molxK	729.81	Joback Method
cpg	1005.42	J/molxK	757.30	Joback Method
cpg	1025.55	J/molxK	784.79	Joback Method
cpg	1044.78	J/molxK	812.28	Joback Method
cpg	1063.16	J/molxK	839.77	Joback Method
cpg	1080.72	J/molxK	867.26	Joback Method
dvisc	0.0040182	Paxs	322.70	Joback Method
dvisc	0.0011754	Paxs	385.97	Joback Method

dvisc	0.0004861	Paxs	449.24	Joback Method
dvisc	0.0002500	Paxs	512.51	Joback Method
dvisc	0.0001488	Paxs	575.78	Joback Method
dvisc	0.0000982	Paxs	639.05	Joback Method
dvisc	0.0000698	Paxs	702.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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