

Hexadecane, 7-methyl-6-pentyl

Inchi:	InChI=1S/C22H46/c1-5-8-11-12-13-14-17-18-21(4)22(19-15-9-6-2)20-16-10-7-3/h21-22H
InchiKey:	KVMXUBFDQJPZHC-UHFFFAOYSA-N
Formula:	C22H46
SMILES:	CCCCCCCCC(C)C(CCCCC)CCCC
Mol. weight [g/mol]:	310.60

Physical Properties

Property code	Value	Unit	Source
gf	129.48	kJ/mol	Joback Method
hf	-507.97	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	63.79	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	8.540		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	2000.00		NIST Webbook
tb	701.88	K	Joback Method
tc	868.08	K	Joback Method
tf	307.70	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.75	J/molxK	701.88	Joback Method
cpg	984.94	J/molxK	729.58	Joback Method
cpg	1006.16	J/molxK	757.28	Joback Method
cpg	1026.44	J/molxK	784.98	Joback Method
cpg	1045.81	J/molxK	812.68	Joback Method
cpg	1064.30	J/molxK	840.38	Joback Method
cpg	1081.95	J/molxK	868.08	Joback Method
dvisc	0.0057276	Paxs	307.70	Joback Method
dvisc	0.0014050	Paxs	373.40	Joback Method

dvisc	0.0005248	Paxs	439.09	Joback Method
dvisc	0.0002533	Paxs	504.79	Joback Method
dvisc	0.0001446	Paxs	570.49	Joback Method
dvisc	0.0000927	Paxs	636.18	Joback Method
dvisc	0.0000646	Paxs	701.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9246&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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