

Hexadecane, 4-octyl

Other names:	Heneicosane, 9-propyl
Inchi:	InChI=1S/C24H50/c1-4-7-9-11-13-14-15-16-18-20-23-24(21-6-3)22-19-17-12-10-8-5-2/h2
InchiKey:	KWVKDYMQYMQAKQ-UHFFFAOYSA-N
Formula:	C24H50
SMILES:	CCCCCCCCCCCC(CCC)CCCCCCC
Mol. weight [g/mol]:	338.65

Physical Properties

Property code	Value	Unit	Source
gf	148.76	kJ/mol	Joback Method
hf	-543.97	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.464		Crippen Method
mcvol	349.020	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	748.08	K	Joback Method
tc	918.22	K	Joback Method
tf	345.24	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.86	J/molxK	748.08	Joback Method
cpg	1110.78	J/molxK	776.44	Joback Method
cpg	1132.66	J/molxK	804.79	Joback Method
cpg	1153.54	J/molxK	833.15	Joback Method
cpg	1173.45	J/molxK	861.51	Joback Method

cpg	1192.43	J/mol×K	889.86	Joback Method
cpg	1210.52	J/mol×K	918.22	Joback Method
dvisc	0.0031119	Paxs	345.24	Joback Method
dvisc	0.0009096	Paxs	412.38	Joback Method
dvisc	0.0003752	Paxs	479.52	Joback Method
dvisc	0.0001924	Paxs	546.66	Joback Method
dvisc	0.0001142	Paxs	613.80	Joback Method
dvisc	0.0000751	Paxs	680.94	Joback Method
dvisc	0.0000532	Paxs	748.08	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=R47746&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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