

Hexadecane, 6,11-dipentyl-

Other names:	6,11-Di-n-pentylhexadecane 6,11-Dipentylhexadecane
Inchi:	InChI=1S/C26H54/c1-5-9-13-19-25(20-14-10-6-2)23-17-18-24-26(21-15-11-7-3)22-16-12
InchiKey:	PNYSRXNTUVFUNI-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCC(CCCCC)CCCC(CCCCC)CCCC
Mol. weight [g/mol]:	366.71
CAS:	15874-03-0

Physical Properties

Property code	Value	Unit	Source
gf	163.16	kJ/mol	Joback Method
hf	-590.53	kJ/mol	Joback Method
hfus	56.05	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	10.100		Crippen Method
mvol	377.200	ml/mol	McGowan Method
pc	731.25	kPa	Joback Method
tb	793.40	K	Joback Method
tc	971.62	K	Joback Method
tf	257.00 ± 0.60	K	NIST Webbook
tf	257.00 ± 2.00	K	NIST Webbook
vc	1.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.80	J/mol×K	971.62	Joback Method
cpg	1217.07	J/mol×K	793.40	Joback Method
cpg	1241.13	J/mol×K	823.10	Joback Method
cpg	1264.02	J/mol×K	852.81	Joback Method
cpg	1285.78	J/mol×K	882.51	Joback Method
cpg	1306.47	J/mol×K	912.22	Joback Method

cpg	1326.13	J/mol×K	941.92	Joback Method
dvisc	0.0000369	Paxs	793.40	Joback Method
dvisc	0.0031975	Paxs	352.78	Joback Method
dvisc	0.0008010	Paxs	426.22	Joback Method
dvisc	0.0003014	Paxs	499.65	Joback Method
dvisc	0.0001457	Paxs	573.09	Joback Method
dvisc	0.0000831	Paxs	646.53	Joback Method
dvisc	0.0000531	Paxs	719.96	Joback Method
hvapt	88.90	kJ/mol	486.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62611e+01
Coeff. B	-6.28969e+03
Coeff. C	-1.28800e+02
Temperature range (K), min.	522.56
Temperature range (K), max.	703.22

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C15874030&Units=SI>

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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