

Hexacosane, 9-octyl-

Other names:	9-Octylhexacosane 9-n-Octylhexacosane
Inchi:	InChI=1S/C34H70/c1-4-7-10-13-16-17-18-19-20-21-22-23-24-27-30-33-34(31-28-25-14-
InchiKey:	CDTWRIBBCOMBSI-UHFFFAOYSA-N
Formula:	C34H70
SMILES:	CCCCCCCCCCCCCCCCCCCC(CCCCCCCC)CCCCCCCC
Mol. weight [g/mol]:	478.92
CAS:	55429-83-9

Physical Properties

Property code	Value	Unit	Source
gf	232.96	kJ/mol	Joback Method
hf	-750.37	kJ/mol	Joback Method
hfus	80.29	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-13.81		Crippen Method
logp	13.365		Crippen Method
mvol	489.920	ml/mol	McGowan Method
pc	499.58	kPa	Joback Method
tb	976.88	K	Joback Method
tc	1226.77	K	Joback Method
tf	296.00 ± 1.00	K	NIST Webbook
vc	1.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1917.55	J/molxK	1226.77	Joback Method
cpg	1894.95	J/molxK	1185.12	Joback Method
cpg	1870.84	J/molxK	1143.48	Joback Method
cpg	1845.07	J/molxK	1101.83	Joback Method
cpg	1817.45	J/molxK	1060.18	Joback Method
cpg	1787.83	J/molxK	1018.53	Joback Method
cpg	1756.03	J/molxK	976.88	Joback Method

dvisc	0.0007325	Paxs	457.94	Joback Method
dvisc	0.0000119	Paxs	976.88	Joback Method
dvisc	0.0000170	Paxs	890.39	Joback Method
dvisc	0.0000261	Paxs	803.90	Joback Method
dvisc	0.0000444	Paxs	717.41	Joback Method
dvisc	0.0000875	Paxs	630.92	Joback Method
dvisc	0.0002138	Paxs	544.43	Joback Method
hvapt	110.30	kJ/mol	556.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50131e+01
Coeff. B	-6.26024e+03
Coeff. C	-1.46870e+02
Temperature range (K), min.	572.00
Temperature range (K), max.	792.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55429839&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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