

Docosane, 7-hexyl-

Other names:	7-Hexyldocosane 7-n-Hexyldocosane
Inchi:	InChI=1S/C28H58/c1-4-7-10-13-14-15-16-17-18-19-20-21-24-27-28(25-22-11-8-5-2)26-2
InchiKey:	SDYSFWMEHHOBQG-UHFFFAOYSA-N
Formula:	C28H58
SMILES:	CCCCCCCCCCCCCCCCCC(CCCCC)CCCCC
Mol. weight [g/mol]:	394.76
CAS:	55373-86-9

Physical Properties

Property code	Value	Unit	Source
gf	182.44	kJ/mol	Joback Method
hf	-626.53	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	11.025		Crippen Method
mvol	405.380	ml/mol	McGowan Method
pc	658.14	kPa	Joback Method
tb	839.60	K	Joback Method
tc	1029.02	K	Joback Method
tf	292.45 ± 0.50	K	NIST Webbook
tf	292.50 ± 2.00	K	NIST Webbook
tf	292.50 ± 1.00	K	NIST Webbook
vc	1.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.34	J/mol×K	839.60	Joback Method
cpg	1373.75	J/mol×K	871.17	Joback Method
cpg	1397.85	J/mol×K	902.74	Joback Method
cpg	1420.68	J/mol×K	934.31	Joback Method
cpg	1442.31	J/mol×K	965.88	Joback Method

cpg	1462.81	J/mol×K	997.45	Joback Method
cpg	1482.23	J/mol×K	1029.02	Joback Method
dvisc	0.0017949	Paxs	390.32	Joback Method
dvisc	0.0005242	Paxs	465.20	Joback Method
dvisc	0.0002154	Paxs	540.08	Joback Method
dvisc	0.0001099	Paxs	614.96	Joback Method
dvisc	0.0000649	Paxs	689.84	Joback Method
dvisc	0.0000425	Paxs	764.72	Joback Method
dvisc	0.0000300	Paxs	839.60	Joback Method
hvapt	100.70	kJ/mol	518.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66252e+01
Coeff. B	-6.64497e+03
Coeff. C	-1.37070e+02
Temperature range (K), min.	543.80
Temperature range (K), max.	724.41

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=C55373869&Units=SI
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/ci990307I

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
h vap:	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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