

Docosane, 9-butyl-

Other names:	9-Butyldocosane 9-n-Butyldocosane
Inchi:	InChI=1S/C26H54/c1-4-7-10-12-14-15-16-17-18-20-22-25-26(23-9-6-3)24-21-19-13-11-8
InchiKey:	OIHDCDZZRDGEIB-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCCCCCCCCC(CCCC)CCCCCCCC
Mol. weight [g/mol]:	366.71
CAS:	55282-14-9

Physical Properties

Property code	Value	Unit	Source
gf	165.60	kJ/mol	Joback Method
hf	-585.25	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	73.08	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	10.244		Crippen Method
mvol	377.200	ml/mol	McGowan Method
pc	728.10	kPa	Joback Method
tb	793.84	K	Joback Method
tc	971.96	K	Joback Method
tf	274.45	K	NIST Webbook
tf	274.50 ± 0.50	K	NIST Webbook
tf	274.50 ± 1.00	K	NIST Webbook
vc	1.486	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.42	J/mol×K	971.96	Joback Method
cpg	1325.72	J/mol×K	942.27	Joback Method
cpg	1306.05	J/mol×K	912.59	Joback Method
cpg	1285.35	J/mol×K	882.90	Joback Method
cpg	1263.59	J/mol×K	853.21	Joback Method

cpg	1240.72	J/mol×K	823.53	Joback Method
cpg	1216.69	J/mol×K	793.84	Joback Method
dvisc	0.0023771	Paxs	367.78	Joback Method
dvisc	0.0000402	Paxs	793.84	Joback Method
dvisc	0.0000568	Paxs	722.83	Joback Method
dvisc	0.0000865	Paxs	651.82	Joback Method
dvisc	0.0001462	Paxs	580.81	Joback Method
dvisc	0.0002858	Paxs	509.80	Joback Method
dvisc	0.0006945	Paxs	438.79	Joback Method
hvapt	91.90	kJ/mol	497.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.68219e+01
Coeff. B	-6.55756e+03
Coeff. C	-1.31677e+02
Temperature range (K), min.	528.28
Temperature range (K), max.	701.38

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/ci990307l>

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=C55282149&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
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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