Docosane, 11-butyl-

Other names: 11-Butyldocosane
11-n-Butyldocosane
Hexadecane, 5-decyl
Inchi: InChI=1S/C26H54/c1-4-7-10-12-14-16-18-20-22-25-26(23-9-6-3)24-21-19-17-15-13-11-8
InchiKey: HEUYLTACOIADBB-UHFFFAOYSA-N
Formula: C26H54
SMILES: CCCCCCCCCCCC(CCCC)CCCCCCCCCC
Mol. weight [g/mol]: 366.71
CAS: 13475-76-8

Physical Properties

Property code	Value	Unit	Source
chl	-17232.60 ± 6.70	kJ/mol	NIST Webbook
gf	165.60	kJ/mol	Joback Method
hf	-593.30 ± 7.50	kJ/mol	NIST Webbook
hfl	-717.60	kJ/mol	NIST Webbook
hfus	59.57	kJ/mol	Joback Method
hvap	123.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-10.46		Crippen Method
logp	10.244		Crippen Method
mcvol	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	273.20 ± 1.00	K	NIST Webbook
tf	273.20 ± 1.00	K	NIST Webbook
tf	273.15	K	NIST Webbook
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.42	J/mol×K	971.96	Joback Method
cpg	1216.69	J/mol×K	793.84	Joback Method

cpg	1240.72	J/mol×K	823.53	Joback Method
cpg	1263.59	J/mol×K	853.21	Joback Method
cpg	1285.35	J/mol×K	882.90	Joback Method
cpg	1306.05	J/mol×K	912.59	Joback Method
cpg	1325.72	J/mol×K	942.27	Joback Method
dvisc	0.0000402	Pa×s	793.84	Joback Method
dvisc	0.0023771	Pa×s	367.78	Joback Method
dvisc	0.0006945	Pa×s	438.79	Joback Method
dvisc	0.0002858	Pa×s	509.80	Joback Method
dvisc	0.0001462	Pa×s	580.81	Joback Method
dvisc	0.0000865	Pa×s	651.82	Joback Method
dvisc	0.0000568	Pa×s	722.83	Joback Method
hvapt	93.30	kJ/mol	498.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	515.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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=C13475768&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume