

Docosane, 5-butyl-

Other names:	5-Butyldocosane 5-n-Butyldocosane
Inchi:	InChI=1S/C26H54/c1-4-7-10-11-12-13-14-15-16-17-18-19-20-21-22-25-26(23-8-5-2)24-9
InchiKey:	CSRNPDQIQWQJCM-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCCCCCCCCCCCCCCC(CCCC)CCCC
Mol. weight [g/mol]:	366.71
CAS:	55282-16-1

Physical Properties

Property code	Value	Unit	Source
chl	-17235.20 ± 6.70	kJ/mol	NIST Webbook
gf	165.60	kJ/mol	Joback Method
hf	-587.40 ± 7.50	kJ/mol	NIST Webbook
hfl	-715.50	kJ/mol	NIST Webbook
hfus	59.57	kJ/mol	Joback Method
hvap	126.00 ± 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	294.00 ± 0.50	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/molxK	823.53	Joback Method
cpg	1216.69	J/molxK	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	94.00	kJ/mol	500.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	517.20	K	1.30	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

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=C55282161&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/ci9903071

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
mccvol:	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

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