

5-Methyldocosane

Other names:	Docosane, 5-methyl
Inchi:	InChI=1S/C23H48/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-23(3)21-7-5-2/h23H
InchiKey:	KDLUJNFDZQOZLK-UHFFFAOYSA-N
Formula:	C23H48
SMILES:	CCCCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	324.63
CAS:	25163-52-4

Physical Properties

Property code	Value	Unit	Source
gf	140.34	kJ/mol	Joback Method
hf	-523.33	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	9.074		Crippen Method
mcvol	334.930	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2253.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	725.20	K	Joback Method
tc	892.42	K	Joback Method
tf	333.97	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.09	J/molxK	892.42	Joback Method
cpg	1024.67	J/molxK	725.20	Joback Method
cpg	1047.11	J/molxK	753.07	Joback Method
cpg	1068.56	J/molxK	780.94	Joback Method
cpg	1089.04	J/molxK	808.81	Joback Method

cpg	1108.60	J/mol×K	836.68	Joback Method
cpg	1127.28	J/mol×K	864.55	Joback Method
dvisc	0.0000611	Paxs	725.20	Joback Method
dvisc	0.0035428	Paxs	333.97	Joback Method
dvisc	0.0010359	Paxs	399.17	Joback Method
dvisc	0.0004278	Paxs	464.38	Joback Method
dvisc	0.0002197	Paxs	529.59	Joback Method
dvisc	0.0001306	Paxs	594.79	Joback Method
dvisc	0.0000860	Paxs	659.99	Joback Method
hvapt	75.60	kJ/mol	568.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.87881e+01
Coeff. B	-9.13136e+03
Coeff. C	1.20800e+00
Temperature range (K), min.	492.37
Temperature range (K), max.	676.36

Sources

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=C25163524&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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