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: CCCCCCCCCCCCCCCCCC(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	2252.00		NIST Webbook
rinpol	2253.00		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	1024.67	J/mol×K	725.20	Joback Method
cpg	1047.11	J/mol×K	753.07	Joback Method
cpg	1068.56	J/mol×K	780.94	Joback Method
cpg	1089.04	J/mol×K	808.81	Joback Method
cpg	1108.60	J/mol×K	836.68	Joback Method

cpg	1127.28	J/mol×K	864.55	Joback Method
cpg	1145.09	J/mol×K	892.42	Joback Method
dvisc	0.0035428	Pa×s	333.97	Joback Method
dvisc	0.0010359	Pa×s	399.17	Joback Method
dvisc	0.0004278	Pa×s	464.38	Joback Method
dvisc	0.0002197	Pa×s	529.59	Joback Method
dvisc	0.0001306	Pa×s	594.79	Joback Method
dvisc	0.0000860	Pa×s	659.99	Joback Method
dvisc	0.0000611	Pa×s	725.20	Joback Method
hvapt	75.60	kJ/mol	568.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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

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

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