Heneicosane, 5-methyl-

Other names:	5-Methylheneicosane
	5-Methylhenicosane
Inchi:	InChI=1S/C22H46/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-21-22(3)20-7-5-2/h22H,4-
InchiKey:	CCXNGHAFWSFYNV-UHFFFAOYSA-N
Formula:	C22H46
SMILES:	CCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	310.60
CAS:	25117-37-7

Physical Properties

Property code	Value	Unit	Source
gf	131.92	kJ/mol	Joback Method
hf	-502.69	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2151.10		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2153.20		NIST Webbook
rinpol	2146.40		NIST Webbook
rinpol	2153.00		NIST Webbook
ripol	2148.50		NIST Webbook
tb	702.32	K	Joback Method
tc	867.26	K	Joback Method
tf	322.70	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.72	J/mol×K	867.26	Joback Method
cpg	1063.16	J/mol×K	839.77	Joback Method
cpg	1044.78	J/mol×K	812.28	Joback Method
cpg	1025.55	J/mol×K	784.79	Joback Method
cpg	1005.42	J/mol×K	757.30	Joback Method
cpg	984.38	J/mol×K	729.81	Joback Method
cpg	962.39	J/mol×K	702.32	Joback Method
dvisc	0.0040182	Pa×s	322.70	Joback Method
dvisc	0.0000698	Pa×s	702.32	Joback Method
dvisc	0.0000982	Pa×s	639.05	Joback Method
dvisc	0.0001488	Pa×s	575.78	Joback Method
dvisc	0.0002500	Pa×s	512.51	Joback Method
dvisc	0.0004861	Pa×s	449.24	Joback Method
dvisc	0.0011754	Pa×s	385.97	Joback Method
hvapt	73.90	kJ/mol	557.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.88529e+01
Coeff. B	-9.07172e+03
Coeff. C	5.15000e+00
Temperature range (K), min.	483.49
Temperature range (K), max.	664.78

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=C25117377&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume