

Heneicosane, 3-methyl-

Other names:	3-Methylheneicosane 3-Methylhenicosane
Inchi:	InChI=1S/C22H46/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(3)5-2/h22H,4-
InchiKey:	OSJUENOXPFHOLF-UHFFFAOYSA-N
Formula:	C22H46
SMILES:	CCCCCCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]:	310.60
CAS:	6418-47-9

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	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2174.30		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2168.50		NIST Webbook
rinpol	2171.30		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2174.00		NIST Webbook
ripol	2169.30		NIST Webbook
tb	702.32	K	Joback Method
tc	867.26	K	Joback Method
tf	292.80 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.39	J/molxK	702.32	Joback Method
cpg	984.38	J/molxK	729.81	Joback Method
cpg	1005.42	J/molxK	757.30	Joback Method
cpg	1025.55	J/molxK	784.79	Joback Method
cpg	1044.78	J/molxK	812.28	Joback Method
cpg	1063.16	J/molxK	839.77	Joback Method
cpg	1080.72	J/molxK	867.26	Joback Method
dvisc	0.0040182	Paxs	322.70	Joback Method
dvisc	0.0011754	Paxs	385.97	Joback Method
dvisc	0.0004861	Paxs	449.24	Joback Method
dvisc	0.0002500	Paxs	512.51	Joback Method
dvisc	0.0001488	Paxs	575.78	Joback Method
dvisc	0.0000982	Paxs	639.05	Joback Method
dvisc	0.0000698	Paxs	702.32	Joback Method
hvapt	74.40	kJ/mol	557.50	NIST Webbook

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=C6418479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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