

Pentadecane, 2,6,10,14-tetramethyl-

Other names:

2,6,10,14-tetramethylpentadecane
2,6,10,14-Tetramethylpentadecane
2,6,10,14-Tetramethylpentadecane (pristane)
Bute hydrocarbon
Norphytan
Norphytane
Norphytane, robuoy
Pristan
Pristane

Inchi:

InChI=1S/C19H40/c1-16(2)10-7-12-18(5)14-9-15-19(6)13-8-11-17(3)4/h16-19H,7-15H2,1

InchiKey:

XOJVVFBDXDTEG-UHFFFAOYSA-N

Formula:

C19H40

SMILES:

CC(C)CCCC(C)CCCC(C)CCCC(C)C

Mol. weight [g/mol]:

268.52

CAS:

1921-70-6

Physical Properties

Property code	Value	Unit	Source
gf	99.34	kJ/mol	Joback Method
hf	-456.61	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	7.082		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1681.90		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1685.00		NIST Webbook

rinpol	1685.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1688.00	NIST Webbook
rinpol	1692.00	NIST Webbook
rinpol	1703.00	NIST Webbook
rinpol	1712.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1708.00	NIST Webbook
rinpol	1703.70	NIST Webbook
rinpol	1703.00	NIST Webbook
rinpol	1702.00	NIST Webbook
rinpol	1712.00	NIST Webbook
rinpol	1701.00	NIST Webbook
rinpol	1696.00	NIST Webbook
rinpol	1704.00	NIST Webbook
rinpol	1682.00	NIST Webbook
rinpol	1649.00	NIST Webbook
rinpol	1705.00	NIST Webbook
rinpol	1703.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1684.00	NIST Webbook
rinpol	1692.00	NIST Webbook
rinpol	1709.00	NIST Webbook
rinpol	1709.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1712.00	NIST Webbook
rinpol	283.84	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1703.00	NIST Webbook
rinpol	1709.00	NIST Webbook
rinpol	1708.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1707.00	NIST Webbook
rinpol	1709.00	NIST Webbook
rinpol	288.01	NIST Webbook
rinpol	1708.00	NIST Webbook
rinpol	1685.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1668.00	NIST Webbook
ripol	1664.00	NIST Webbook

ripol	1669.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	632.36	K	Joback Method
tc	799.95	K	Joback Method
tf	173.20 ± 10.00	K	NIST Webbook
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.42	J/molxK	799.95	Joback Method
cpg	882.11	J/molxK	772.02	Joback Method
cpg	863.98	J/molxK	744.09	Joback Method
cpg	844.99	J/molxK	716.16	Joback Method
cpg	825.12	J/molxK	688.22	Joback Method
cpg	804.34	J/molxK	660.29	Joback Method
cpg	782.62	J/molxK	632.36	Joback Method
cpl	569.76	J/molxK	298.15	NIST Webbook
dvisc	0.0001233	Paxs	567.62	Joback Method
dvisc	0.0002055	Paxs	502.87	Joback Method
dvisc	0.0003981	Paxs	438.12	Joback Method
dvisc	0.0009702	Paxs	373.38	Joback Method
dvisc	0.0034361	Paxs	308.63	Joback Method
dvisc	0.0238146	Paxs	243.89	Joback Method
dvisc	0.0000822	Paxs	632.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52108e+01
Coeff. B	-4.97608e+03
Coeff. C	-9.93740e+01
Temperature range (K), min.	432.82
Temperature range (K), max.	602.04

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1921706&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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