

Hexacosane, 3-methyl

Inchi:

InChI=1S/C27H56/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27

InchiKey:

YMQJCTWHHRBBQA-UHFFFAOYSA-N

Formula:

C27H56

SMILES:

CCCCCCCCCCCCCCCCCCCCCCCC(C)CC

Mol. weight [g/mol]:

380.73

CAS:

65820-56-6

Physical Properties

Property code	Value	Unit	Source
gf	174.02	kJ/mol	Joback Method
hf	-605.89	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-10.88		Crippen Method
logp	10.635		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2672.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2672.00		NIST Webbook
rinpol	2673.40		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2675.70		NIST Webbook
rinpol	2665.00		NIST Webbook
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook
rinpol	2675.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	816.72	K	Joback Method
tc	1000.04	K	Joback Method
tf	379.05	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.19	J/mol×K	816.72	Joback Method
cpg	1393.80	J/mol×K	969.49	Joback Method
cpg	1373.74	J/mol×K	938.93	Joback Method
cpg	1352.60	J/mol×K	908.38	Joback Method
cpg	1330.33	J/mol×K	877.83	Joback Method
cpg	1306.88	J/mol×K	847.27	Joback Method
cpg	1412.85	J/mol×K	1000.04	Joback Method
dvisc	0.0000347	Pa×s	816.72	Joback Method
dvisc	0.0000492	Pa×s	743.77	Joback Method
dvisc	0.0000750	Pa×s	670.83	Joback Method
dvisc	0.0001269	Pa×s	597.88	Joback Method
dvisc	0.0002484	Pa×s	524.94	Joback Method
dvisc	0.0006041	Pa×s	451.99	Joback Method
dvisc	0.0020683	Pa×s	379.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65820566&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical 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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