Hexacosane, 11-methyl

Other names: Hexacosane, 11-methyl
Inchi: InChI=1S/C27H56/c1-4-6-8-10-12-14-15-16-17-18-20-22-24-26-27(3)25-23-21-19-13-11-
InchiKey: ATFOATQSPLHNOV-UHFFFAOYSA-N
Formula: C27H56
SMILES: CCCCCCCCCCCCCCCC(C)CCCCCCCCCC
Mol. weight [g/mol]: 380.74

Physical Properties

Property code	Value	Unit	Source
af	1.0614		Cheméo Relay (1.0)
gf	174.02	kJ/mol	Joback Method
hf	-612.36	kJ/mol	Cheméo Relay (1.0)
hfus	62.16	kJ/mol	Joback Method
hvap	131.14	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-10.48		Cheméo Relay (1.0)
logp	10.635		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2636.30		NIST Webbook
rinpol	2632.00		NIST Webbook
rinpol	2634.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2636.30		NIST Webbook
tb	620.23	K	Cheméo Relay (1.0)
tc	792.17	K	Cheméo Relay (1.0)
tf	294.41	K	Cheméo Relay (1.0)
vc	1.544	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.19	J/mol×K	816.72	Joback Method

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261800&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

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

ie: Ionization energy

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