2-methylhexacosane

Inchi: InChI=1S/C27H56/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: BEBPORIYFVRVCP-UHFFFAOYSA-N
Formula: C27H56
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 380.74
CAS: 1561-02-0

Physical Properties

Property code	Value	Unit	Source
af	1.0759		Cheméo Relay (1.0)
gf	174.02	kJ/mol	Joback Method
hf	-619.54	kJ/mol	Cheméo Relay (1.0)
hfus	62.16	kJ/mol	Joback Method
hvap	133.34	kJ/mol	Cheméo Relay (1.0)
ie	10.12	eV	Cheméo Relay (1.0)
log10ws	-10.53		Cheméo Relay (1.0)
logp	10.635		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2664.00		NIST Webbook
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
rinpol	2664.00		NIST Webbook
rinpol	2665.30		NIST Webbook
rinpol	2664.00		NIST Webbook
rinpol	2664.00		NIST Webbook
rinpol	2662.70		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	622.38	K	Cheméo Relay (1.0)
tc	791.03	K	Cheméo Relay (1.0)
tf	315.48	K	Cheméo Relay (1.0)
vc	1.564	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
hvapt	109.60	kJ/mol	565.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47342e+01
Coeff. B	-5.29618e+03
Coeff. C	-1.66850e+02
Temperature range (K), min.	533.45
Temperature range (K), max.	728.91

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1561020&Units=SI

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

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume