Pentacosane, 13-undecyl-

Other names:	13-Undecylpentacosane
	13-n-Undecylpentacosane
Inchi:	InChI=1S/C36H74/c1-4-7-10-13-16-19-22-25-28-31-34-36(33-30-27-24-21-18-15-12-9-6-
InchiKey:	ZBOLLHDWYFHOST-UHFFFAOYSA-N
Formula:	C36H74
SMILES:	CCCCCCCCCCCCC(CCCCCCCCCCC)CCCCCCCCCCCC
Mol. weight [g/mol]:	506.97
CAS:	55517-89-0

Physical Properties

Property code	Value	Unit	Source
gf	249.80	kJ/mol	Joback Method
hf	-791.65	kJ/mol	Joback Method
hfus	85.47	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-14.65		Crippen Method
logp	14.146		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	459.31	kPa	Joback Method
tb	1022.64	K	Joback Method
tc	1304.31	K	Joback Method
tf	282.90 ± 1.00	K	NIST Webbook
vc	2.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2069.95	J/mol×K	1304.31	Joback Method
cpg	2045.68	J/mol×K	1257.37	Joback Method
cpg	2019.81	J/mol×K	1210.42	Joback Method
cpg	1992.06	J/mol×K	1163.48	Joback Method
cpg	1962.18	J/mol×K	1116.53	Joback Method
cpg	1929.92	J/mol×K	1069.59	Joback Method
cpg	1895.00	J/mol×K	1022.64	Joback Method

dvisc	0.0005358	Pa×s	480.48	Joback Method
dvisc	0.0000087	Pa×s	1022.64	Joback Method
dvisc	0.0000123	Pa×s	932.28	Joback Method
dvisc	0.0000190	Pa×s	841.92	Joback Method
dvisc	0.0000324	Pa×s	751.56	Joback Method
dvisc	0.0000639	Pa×s	661.20	Joback Method
dvisc	0.0001564	Pa×s	570.84	Joback Method
hvapt	132.90	kJ/mol	564.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57886e+01
Coeff. B	-6.83390e+03
Coeff. C	-1.55252e+02
Temperature range (K), min.	596.12
Temperature range (K), max.	807.52

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517890&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/ci990307l

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

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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume