Pentacosane, 13-phenyl-

Other names:	13-Phenylpentacosane
	Benzene, (1-dodecyltridecyl)-
Inchi:	InChI=1S/C31H56/c1-3-5-7-9-11-13-15-17-19-22-26-30(31-28-24-21-25-29-31)27-23-20-
InchiKey:	FARZSOUCOJBKMW-UHFFFAOYSA-N
Formula:	C31H56
SMILES:	CCCCCCCCCCCCC(CCCCCCCCCCCC)c1ccccc1
Mol. weight [g/mol]:	428.78
CAS:	6006-90-2

Physical Properties

Property code	Value	Unit	Source
chs	-19515.00 ± 7.50	kJ/mol	NIST Webbook
gf	320.11	kJ/mol	Joback Method
hf	-451.92	kJ/mol	Joback Method
hfs	-687.00 ± 7.60	kJ/mol	NIST Webbook
hfus	66.56	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-11.87		Crippen Method
logp	11.392		Crippen Method
mcvol	423.890	ml/mol	McGowan Method
pc	672.90	kPa	Joback Method
tb	934.92	K	Joback Method
tc	1146.15	K	Joback Method
tf	138.10 ± 6.27	K	NIST Webbook
tf	304.85 ± 0.50	K	NIST Webbook
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1582.20	J/mol×K	1146.15	Joback Method
cpg	1564.32	J/mol×K	1110.95	Joback Method
cpg	1545.39	J/mol×K	1075.74	Joback Method
cpg	1525.32	J/mol×K	1040.54	Joback Method

cpg	1504.00	J/mol×K	1005.33	Joback Method
cpg	1481.34	J/mol×K	970.13	Joback Method
cpg	1457.24	J/mol×K	934.92	Joback Method
dvisc	0.0008742	Pa×s	450.55	Joback Method
dvisc	0.0000196	Pa×s	934.92	Joback Method
dvisc	0.0000274	Pa×s	854.19	Joback Method
dvisc	0.0000411	Pa×s	773.46	Joback Method
dvisc	0.0000675	Pa×s	692.73	Joback Method
dvisc	0.0001265	Pa×s	612.01	Joback Method
dvisc	0.0002872	Pa×s	531.28	Joback Method
hvapt	106.70	kJ/mol	527.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39905e+01
Coeff. B	-5.68118e+03
Coeff. C	-1.45522e+02
Temperature range (K), min.	560.12
Temperature range (K), max.	800.11

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6006902&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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