1-Phenylheneicosane

Other names: 11-Phenylheneicosane
Benzene, heneicosyl-
Inchi: InChI=1S/C27H48/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-24-27-25-22-2
InchiKey: OWXCBZFAHWMZCQ-UHFFFAOYSA-N
Formula: C27H48
SMILES: CCCCCCCCCCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]: 372.67
CAS: 40775-09-5

Physical Properties

Property code	Value	Unit	Source
chl	-16977.80 ± 6.70	kJ/mol	NIST Webbook
chl	-16980.80 ± 6.70	kJ/mol	NIST Webbook
gf	288.87	kJ/mol	Joback Method
hf	-364.08	kJ/mol	Joback Method
hfl	-506.80 ± 6.70	kJ/mol	NIST Webbook
hfl	-508.10 ± 6.70	kJ/mol	NIST Webbook
hfus	59.73	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	9.661		Crippen Method
mcvol	367.530	ml/mol	McGowan Method
pc	826.21	kPa	Joback Method
tb	843.84	K	Joback Method
tc	1034.66	K	Joback Method
tf	420.47	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.03	J/mol×K	843.84	Joback Method
cpg	1218.17	J/mol×K	875.64	Joback Method
cpg	1239.09	J/mol×K	907.45	Joback Method

cpg	1258.88	J/mol×K	939.25	Joback Method
cpg	1277.60	J/mol×K	971.05	Joback Method
cpg	1295.31	J/mol×K	1002.85	Joback Method
cpg	1312.07	J/mol×K	1034.66	Joback Method
dvisc	0.0012137	Pa×s	420.47	Joback Method
dvisc	0.0004526	Pa×s	491.03	Joback Method
dvisc	0.0002163	Pa×s	561.59	Joback Method
dvisc	0.0001219	Pa×s	632.15	Joback Method
dvisc	0.0000770	Pa×s	702.72	Joback Method
dvisc	0.0000530	Pa×s	773.28	Joback Method
dvisc	0.0000388	Pa×s	843.84	Joback Method
hvapt	108.40	kJ/mol	575.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40815e+01
Coeff. B	-5.44421e+03
Coeff. C	-1.34916e+02
Temperature range (K), min.	529.60
Temperature range (K), max.	755.69

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40775095&Units=SI

Legend

chl: Standard liquid 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
hfl:	Liquid 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