Benzene, (1-hexadecylheptadecyl)-

Other names: 17-Phenyltritriacontane
Inchi: InChI=1S/C39H72/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-30-34-38(39-36-32-29-33-37-
InchiKey: UZKLDVKDLHPERA-UHFFFAOYSA-N
Formula: C39H72
SMILES: CCCCCCCCCCCCCCCCC(CCCCCCCCCCCCCCCCC)c1ccccc1
Mol. weight [g/mol]: 540.99
CAS: 55517-74-3

Physical Properties

Property code	Value	Unit	Source
gf	387.47	kJ/mol	Joback Method
hf	-617.04	kJ/mol	Joback Method
hfus	87.28	kJ/mol	Joback Method
hvap	104.30	kJ/mol	Joback Method
log10ws	-15.21		Crippen Method
logp	14.513		Crippen Method
mcvol	536.610	ml/mol	McGowan Method
pc	467.90	kPa	Joback Method
tb	1117.96	K	Joback Method
tc	1428.15	K	Joback Method
tf	540.71	K	Joback Method
vc	2.106	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1999.43	J/mol×K	1117.96	Joback Method
cpg	2032.22	J/mol×K	1169.66	Joback Method
cpg	2062.57	J/mol×K	1221.36	Joback Method
cpg	2090.89	J/mol×K	1273.06	Joback Method
cpg	2117.56	J/mol×K	1324.75	Joback Method
cpg	2142.99	J/mol×K	1376.45	Joback Method
cpg	2167.58	J/mol×K	1428.15	Joback Method
dvisc	0.0002665	Pa×s	540.71	Joback Method

dvisc	0.0000859	Pa×s	636.92	Joback Method
dvisc	0.0000372	Pa×s	733.13	Joback Method
dvisc	0.0000196	Pa×s	829.34	Joback Method
dvisc	0.0000118	Pa×s	925.54	Joback Method
dvisc	0.0000078	Pa×s	1021.75	Joback Method
dvisc	0.0000056	Pa×s	1117.96	Joback Method
hvapt	147.10	kJ/mol	557.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29231e+01
Coeff. B	-5.53446e+03
Coeff. C	-1.57990e+02
Temperature range (K), min.	596.00
Temperature range (K), max.	885.10

Sources

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=C55517743&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

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