

Benzene, (1-methylpentadecyl)-

Other names:	Hexadecane, 2-phenyl- 2-phenylhexadecane
Inchi:	InChI=1S/C22H38/c1-3-4-5-6-7-8-9-10-11-12-13-15-18-21(2)22-19-16-14-17-20-22/h14,15,16,17,18,19,20,21,22
InchiKey:	ZUXDORPHXZKYTN-UHFFFAOYSA-N
Formula:	C22H38
SMILES:	CCCCCCCCCCCCCCC(C)c1ccccc1
Mol. weight [g/mol]:	302.54
CAS:	13419-16-4

Physical Properties

Property code	Value	Unit	Source
gf	244.33	kJ/mol	Joback Method
hf	-266.16	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.881		Crippen Method
mvol	297.080	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
tb	729.00	K	Joback Method
tc	913.46	K	Joback Method
tf	349.12	K	Joback Method
vc	1.153	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.61	J/mol×K	729.00	Joback Method
cpg	906.56	J/mol×K	759.74	Joback Method
cpg	926.42	J/mol×K	790.49	Joback Method
cpg	945.23	J/mol×K	821.23	Joback Method
cpg	963.04	J/mol×K	851.97	Joback Method
cpg	979.90	J/mol×K	882.72	Joback Method
cpg	995.86	J/mol×K	913.46	Joback Method

dvisc	0.0027423	Paxs	349.12	Joback Method
dvisc	0.0009325	Paxs	412.43	Joback Method
dvisc	0.0004225	Paxs	475.75	Joback Method
dvisc	0.0002306	Paxs	539.06	Joback Method
dvisc	0.0001429	Paxs	602.37	Joback Method
dvisc	0.0000970	Paxs	665.69	Joback Method
dvisc	0.0000704	Paxs	729.00	Joback Method

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=C13419164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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