

Benzene, (1-hexyl-1-heptenyl)-

Other names:	7-Phenyl-6-tridecene
Inchi:	InChI=1S/C19H30/c1-3-5-7-10-14-18(15-11-8-6-4-2)19-16-12-9-13-17-19/h9,12-14,16-17
InchiKey:	FJAXETQQGPFGLT-NBVRZTHBSA-N
Formula:	C19H30
SMILES:	<chem>CCCCCC=C(CCCCCC)c1ccccc1</chem>
Mol. weight [g/mol]:	258.44
CAS:	55030-46-1

Physical Properties

Property code	Value	Unit	Source
gf	293.18	kJ/mol	Joback Method
hf	-91.53	kJ/mol	Joback Method
hfus	37.90	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.621		Crippen Method
mcvol	250.510	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
tb	664.84	K	Joback Method
tc	857.78	K	Joback Method
tf	311.27	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.11	J/mol×K	664.84	Joback Method
cpg	707.98	J/mol×K	697.00	Joback Method
cpg	726.77	J/mol×K	729.15	Joback Method
cpg	744.54	J/mol×K	761.31	Joback Method
cpg	761.34	J/mol×K	793.47	Joback Method
cpg	777.24	J/mol×K	825.63	Joback Method
cpg	792.29	J/mol×K	857.78	Joback Method
hvapt	77.20	kJ/mol	420.00	NIST Webbook

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=C55030461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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