

Benzene, (1-hexylheptyl)-

Other names:	Tridecane, 7-phenyl- 7-Phenyltridecane
Inchi:	InChI=1S/C19H32/c1-3-5-7-10-14-18(15-11-8-6-4-2)19-16-12-9-13-17-19/h9,12-13,16-18
InchiKey:	IMXZNWPPLCVUDT-UHFFFAOYSA-N
Formula:	C19H32
SMILES:	CCCCCCCC(CCCCCC)c1ccccc1
Mol. weight [g/mol]:	260.46
CAS:	2400-01-3

Physical Properties

Property code	Value	Unit	Source
gf	219.07	kJ/mol	Joback Method
hf	-204.24	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Joback Method
ie	8.90 ± 0.10	eV	NIST Webbook
log10ws	-6.84		Crippen Method
logp	6.711		Crippen Method
mcvol	254.810	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	308.30		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1813.00		NIST Webbook
tb	660.36	K	Joback Method
tc	847.35	K	Joback Method
tf	244.95 ± 0.50	K	NIST Webbook
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.11	J/mol×K	847.35	Joback Method
cpg	710.04	J/mol×K	660.36	Joback Method
cpg	730.40	J/mol×K	691.52	Joback Method

cpg	749.69	J/mol×K	722.69	Joback Method
cpg	767.96	J/mol×K	753.85	Joback Method
cpg	785.26	J/mol×K	785.02	Joback Method
cpg	801.63	J/mol×K	816.18	Joback Method
dvisc	0.0001019	Pa×s	660.36	Joback Method
dvisc	0.0037196	Pa×s	315.31	Joback Method
dvisc	0.0012862	Pa×s	372.82	Joback Method
dvisc	0.0005907	Pa×s	430.33	Joback Method
dvisc	0.0003259	Pa×s	487.84	Joback Method
dvisc	0.0002039	Pa×s	545.34	Joback Method
dvisc	0.0001395	Pa×s	602.85	Joback Method
hvapt	76.20	kJ/mol	441.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2400013&Units=SI
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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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