

Benzene, (1-butylnonyl)-

Other names:	Tridecane, 5-phenyl-
Inchi:	InChI=1S/C19H32/c1-3-5-7-8-9-11-15-18(14-6-4-2)19-16-12-10-13-17-19/h10,12-13,16-1
InchiKey:	MZTIRLOLMGVVEK-UHFFFAOYSA-N
Formula:	C19H32
SMILES:	CCCCCCCCC(CCCC)c1ccccc1
Mol. weight [g/mol]:	260.46
CAS:	4534-50-3

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
log10ws	-6.84		Crippen Method
logp	6.711		Crippen Method
mcvol	254.810	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	309.50		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	309.50		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
ripol	2026.00		NIST Webbook
tb	660.36	K	Joback Method
tc	847.35	K	Joback Method
tf	315.31	K	Joback Method
vc	0.986	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	710.04	J/molxK	660.36	Joback Method
cpg	730.40	J/molxK	691.52	Joback Method
cpg	749.69	J/molxK	722.69	Joback Method
cpg	767.96	J/molxK	753.85	Joback Method
cpg	785.26	J/molxK	785.02	Joback Method
cpg	801.63	J/molxK	816.18	Joback Method
cpg	817.11	J/molxK	847.35	Joback Method
dvisc	0.0037196	Paxs	315.31	Joback Method
dvisc	0.0012862	Paxs	372.82	Joback Method
dvisc	0.0005907	Paxs	430.33	Joback Method
dvisc	0.0003259	Paxs	487.84	Joback Method
dvisc	0.0002039	Paxs	545.34	Joback Method
dvisc	0.0001395	Paxs	602.85	Joback Method
dvisc	0.0001019	Paxs	660.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4534503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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