

Benzene, (1-butylheptyl)-

Other names:	Undecane, 5-phenyl-
Inchi:	InChI=1S/C17H28/c1-3-5-7-9-13-16(12-6-4-2)17-14-10-8-11-15-17/h8,10-11,14-16H,3-7,
InchiKey:	RRPCXIBGXYGQNC-UHFFFAOYSA-N
Formula:	C17H28
SMILES:	CCCCCCCC(CCCC)c1ccccc1
Mol. weight [g/mol]:	232.40
CAS:	4537-15-9

Physical Properties

Property code	Value	Unit	Source
gf	202.23	kJ/mol	Joback Method
hf	-162.96	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.931		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	278.70		NIST Webbook
rinpol	278.70		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1628.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1828.00		NIST Webbook
tb	614.60	K	Joback Method
tc	805.23	K	Joback Method
tf	292.77	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.76	J/mol×K	614.60	Joback Method
cpg	618.59	J/mol×K	646.37	Joback Method
cpg	637.37	J/mol×K	678.14	Joback Method
cpg	655.16	J/mol×K	709.91	Joback Method
cpg	671.98	J/mol×K	741.69	Joback Method
cpg	687.89	J/mol×K	773.46	Joback Method
cpg	702.92	J/mol×K	805.23	Joback Method
dvisc	0.0044125	Pa×s	292.77	Joback Method
dvisc	0.0015465	Pa×s	346.41	Joback Method
dvisc	0.0007180	Pa×s	400.05	Joback Method
dvisc	0.0003996	Pa×s	453.69	Joback Method
dvisc	0.0002518	Pa×s	507.32	Joback Method
dvisc	0.0001733	Pa×s	560.96	Joback Method
dvisc	0.0001273	Pa×s	614.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4537159&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
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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