

Benzene, (1-butyloctyl)-

Other names:	Dodecane, 5-phenyl- 5-Phenyldodecane
Inchi:	InChI=1S/C18H30/c1-3-5-7-8-10-14-17(13-6-4-2)18-15-11-9-12-16-18/h9,11-12,15-17H,3
InchiKey:	NPAWGLOPXKCTCV-UHFFFAOYSA-N
Formula:	C18H30
SMILES:	CCCCCCCC(CCCC)c1ccccc1
Mol. weight [g/mol]:	246.43
CAS:	2719-63-3

Physical Properties

Property code	Value	Unit	Source
gf	210.65	kJ/mol	Joback Method
hf	-183.60	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	6.321		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	293.70		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1722.00		NIST Webbook
ripol	1928.00		NIST Webbook
tb	637.48	K	Joback Method
tc	826.13	K	Joback Method
tf	304.04	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.77	J/molxK	637.48	Joback Method
cpg	673.88	J/molxK	668.92	Joback Method
cpg	692.94	J/molxK	700.36	Joback Method
cpg	710.99	J/molxK	731.80	Joback Method
cpg	728.07	J/molxK	763.24	Joback Method
cpg	744.23	J/molxK	794.68	Joback Method
cpg	759.51	J/molxK	826.13	Joback Method
dvisc	0.0040664	Paxs	304.04	Joback Method
dvisc	0.0014152	Paxs	359.61	Joback Method
dvisc	0.0006534	Paxs	415.19	Joback Method
dvisc	0.0003620	Paxs	470.76	Joback Method
dvisc	0.0002272	Paxs	526.33	Joback Method
dvisc	0.0001559	Paxs	581.91	Joback Method
dvisc	0.0001142	Paxs	637.48	Joback Method

Sources

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=C2719633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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