

Benzene, 1-butyl-2,3-dimethyl

Inchi:	InChI=1S/C12H18/c1-4-5-8-12-9-6-7-10(2)11(12)3/h6-7,9H,4-5,8H2,1-3H3
InchiKey:	YFRGOBSBDSYRNN-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCCc1cccc(C)c1C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	143.31	kJ/mol	Joback Method
hf	-77.42	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	45.91	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.646		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	510.60	K	Joback Method
tc	712.18	K	Joback Method
tf	276.46	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.80	J/molxK	510.60	Joback Method
cpg	362.94	J/molxK	544.20	Joback Method
cpg	378.30	J/molxK	577.79	Joback Method
cpg	392.88	J/molxK	611.39	Joback Method
cpg	406.73	J/molxK	644.99	Joback Method
cpg	419.85	J/molxK	678.59	Joback Method
cpg	432.28	J/molxK	712.18	Joback Method

dvisc	0.0018797	Paxs	276.46	Joback Method
dvisc	0.0010177	Paxs	315.48	Joback Method
dvisc	0.0006307	Paxs	354.51	Joback Method
dvisc	0.0004298	Paxs	393.53	Joback Method
dvisc	0.0003139	Paxs	432.55	Joback Method
dvisc	0.0002414	Paxs	471.58	Joback Method
dvisc	0.0001933	Paxs	510.60	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=R52925&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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