

Benzene, (1-ethyl-2-methylpropyl)

Inchi:	InChI=1S/C12H18/c1-4-12(10(2)3)11-8-6-5-7-9-11/h5-10,12H,4H2,1-3H3
InchiKey:	KXKQNZYTNYNPED-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCC(c1ccccc1)C(C)C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	157.69	kJ/mol	Joback Method
hf	-65.04	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.836		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
ripol	1367.00		NIST Webbook
tb	499.76	K	Joback Method
tc	708.09	K	Joback Method
tf	221.42	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.83	J/molxK	499.76	Joback Method
cpg	363.63	J/molxK	534.48	Joback Method
cpg	380.42	J/molxK	569.20	Joback Method
cpg	396.25	J/molxK	603.93	Joback Method
cpg	411.16	J/molxK	638.65	Joback Method
cpg	425.18	J/molxK	673.37	Joback Method
cpg	438.35	J/molxK	708.09	Joback Method
dvisc	0.0091404	Paxs	221.42	Joback Method
dvisc	0.0027198	Paxs	267.81	Joback Method

dvisc	0.0011576	Paxs	314.20	Joback Method
dvisc	0.0006138	Paxs	360.59	Joback Method
dvisc	0.0003761	Paxs	406.98	Joback Method
dvisc	0.0002548	Paxs	453.37	Joback Method
dvisc	0.0001855	Paxs	499.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R539450&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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