

Benzene, (3,3-dimethylbutyl)-

Other names:	(3,3-Dimethylbutyl)benzene
Inchi:	InChI=1S/C12H18/c1-12(2,3)10-9-11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3
InchiKey:	NKDJZTYRVIGJCG-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CC(C)(C)CCc1ccccc1
Mol. weight [g/mol]:	162.27
CAS:	17314-92-0

Physical Properties

Property code	Value	Unit	Source
gf	165.41	kJ/mol	Joback Method
hf	-63.23	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	43.29	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.665		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	485.00 ± 4.00	K	NIST Webbook
tc	709.64	K	Joback Method
tf	253.84	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.23	J/mol×K	497.41	Joback Method
cpg	428.43	J/mol×K	674.27	Joback Method
cpg	414.48	J/mol×K	638.90	Joback Method
cpg	399.55	J/mol×K	603.52	Joback Method
cpg	383.57	J/mol×K	568.15	Joback Method
cpg	366.48	J/mol×K	532.78	Joback Method
cpg	441.46	J/mol×K	709.64	Joback Method
dvisc	0.0002010	Pa×s	497.41	Joback Method

dvisc	0.0002730	Pa×s	456.81	Joback Method
dvisc	0.0003937	Pa×s	416.22	Joback Method
dvisc	0.0006144	Pa×s	375.62	Joback Method
dvisc	0.0010682	Pa×s	335.03	Joback Method
dvisc	0.0021629	Pa×s	294.44	Joback Method
dvisc	0.0054882	Pa×s	253.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17314920&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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