Benzene, (2,2-dimethylpropyl)-

Other names:	(2,2-dimethylpropyl)benzene
	2,2-Dimethyl-1-phenylpropane
	2,2-dimethylpropylbenzene
	Benzene, neopentyl-
	Neopentylbenzene
	t-Pentylbenzene
Inchi:	InChI=1S/C11H16/c1-11(2,3)9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	CJGXJKVMUHXVHL-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CC(C)(C)Cc1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	1007-26-7

Physical Properties

Property code	Value	Unit	Source
gf	156.99	kJ/mol	Joback Method
hf	-42.59	kJ/mol	Joback Method
hfus	15.38	kJ/mol	Thermodynamic properties of neopentylbenzene over the range from T approaching (0 to 350) K
hvap	41.06	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.41 ± 0.04	eV	NIST Webbook
log10ws	-4.15		Aqueous Solubility Prediction Method
log10ws	-4.15		Estimated Solubility Method
logp	3.275		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1040.69		NIST Webbook
rinpol	1068.02		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1058.00		NIST Webbook

rinpol	1049.08		NIST Webbook
rinpol	1052.19		NIST Webbook
rinpol	1060.23		NIST Webbook
rinpol	1064.88		NIST Webbook
rinpol	1068.02		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1040.69		NIST Webbook
tb	458.70	K	NIST Webbook
tb	457.50 ± 0.50	K	NIST Webbook
tb	459.00 ± 4.00	K	NIST Webbook
tc	690.01	K	Joback Method
tf	242.57	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.58	J/mol×K	474.53	Joback Method
cpg	320.10	J/mol×K	510.44	Joback Method
cpg	336.48	J/mol×K	546.36	Joback Method
cpg	351.76	J/mol×K	582.27	Joback Method
cpg	366.02	J/mol×K	618.19	Joback Method
cpg	379.31	J/mol×K	654.10	Joback Method
cpg	391.69	J/mol×K	690.01	Joback Method
dvisc	0.0056791	Pa×s	242.57	Joback Method
dvisc	0.0022674	Pa×s	281.23	Joback Method
dvisc	0.0011302	Pa×s	319.89	Joback Method
dvisc	0.0006546	Pa×s	358.55	Joback Method
dvisc	0.0004217	Pa×s	397.21	Joback Method
dvisc	0.0002937	Pa×s	435.87	Joback Method
dvisc	0.0002169	Pa×s	474.53	Joback Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of neopentylbenzene over the range from T approaching (0 to 350) K:	https://www.doi.org/10.1016/j.jct.2011.12.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
ie:	Ionization energy
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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