Benzene, (1,1-dimethylbutyl)-

Other names: (1,1-Dimethylbutyl)benzene
2-Methyl-2-phenylpentane
Inchi: InChI=1S/C12H18/c1-4-10-12(2,3)11-8-6-5-7-9-11/h5-9H,4,10H2,1-3H3
InchiKey: PIUUDKDOAUICQP-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCC(C)(C)c1ccccc1
Mol. weight [g/mol]: 162.27
CAS: 1985-57-5

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	-3.62		Crippen Method
logp	3.764		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1378.00		NIST Webbook
tb	497.41	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47354e+01
Coeff. B	-4.09168e+03
Coeff. C	-7.42150e+01
Temperature range (K), min.	357.42
Temperature range (K), max.	508.40

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=C1985575&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor 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