

Benzylcyclobutane

Other names:	cyclobutylphenylmethane
Inchi:	InChI=1S/C11H14/c1-2-5-10(6-3-1)9-11-7-4-8-11/h1-3,5-6,11H,4,7-9H2
InchiKey:	VCFOCJUHWQFXBR-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	c1ccc(CC2CCC2)cc1
Mol. weight [g/mol]:	146.23
CAS:	5244-88-2

Physical Properties

Property code	Value	Unit	Source
gf	202.80	kJ/mol	Joback Method
hf	32.80	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	42.44	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.029		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	488.77	K	Joback Method
tc	715.86	K	Joback Method
tf	254.57	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.56	J/mol×K	488.77	Joback Method
cpg	303.94	J/mol×K	526.62	Joback Method
cpg	321.05	J/mol×K	564.47	Joback Method
cpg	336.98	J/mol×K	602.31	Joback Method
cpg	351.78	J/mol×K	640.16	Joback Method
cpg	365.53	J/mol×K	678.01	Joback Method
cpg	378.30	J/mol×K	715.86	Joback Method
dvisc	0.0026703	Pa×s	254.57	Joback Method

dvisc	0.0015215	Pa×s	293.60	Joback Method
dvisc	0.0009892	Pa×s	332.64	Joback Method
dvisc	0.0007040	Pa×s	371.67	Joback Method
dvisc	0.0005345	Pa×s	410.70	Joback Method
dvisc	0.0004257	Pa×s	449.74	Joback Method
dvisc	0.0003516	Pa×s	488.77	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=C5244882&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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