

Cyclooctane, butyl-

Inchi:	InChI=1S/C12H24/c1-2-3-9-12-10-7-5-4-6-8-11-12/h12H,2-11H2,1H3
InchiKey:	MBACTSHRHMTZMA-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CCCCC1CCCCCCC1
Mol. weight [g/mol]:	168.32
CAS:	16538-93-5

Physical Properties

Property code	Value	Unit	Source
gf	50.41	kJ/mol	Joback Method
hf	-249.01	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	43.08	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.537		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
tb	502.05	K	Joback Method
tc	708.87	K	Joback Method
tf	225.34	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.78	J/molxK	502.05	Joback Method
cpg	419.93	J/molxK	536.52	Joback Method
cpg	441.93	J/molxK	570.99	Joback Method
cpg	462.79	J/molxK	605.46	Joback Method
cpg	482.53	J/molxK	639.93	Joback Method
cpg	501.18	J/molxK	674.40	Joback Method
cpg	518.75	J/molxK	708.87	Joback Method
dvisc	0.0204468	Paxs	225.34	Joback Method
dvisc	0.0045561	Paxs	271.46	Joback Method

dvisc	0.0015701	Paxs	317.58	Joback Method
dvisc	0.0007090	Paxs	363.69	Joback Method
dvisc	0.0003828	Paxs	409.81	Joback Method
dvisc	0.0002342	Paxs	455.93	Joback Method
dvisc	0.0001568	Paxs	502.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16538935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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