

Cyclopropane, butyl-

Other names:	Butane, 1-cyclopropyl- Butylcyclopropane
Inchi:	InChI=1S/C7H14/c1-2-3-4-7-5-6-7/h7H,2-6H2,1H3
InchiKey:	SXZVSSJONMPJMN-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCCCC1CC1
Mol. weight [g/mol]:	98.19
CAS:	930-57-4

Physical Properties

Property code	Value	Unit	Source
gf	68.81	kJ/mol	Joback Method
hf	-115.01	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	31.09	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.587		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	712.50		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	713.70		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	714.00		NIST Webbook
tb	372.70 ± 0.60	K	NIST Webbook
tb	371.15 ± 1.50	K	NIST Webbook
tb	372.70 ± 0.50	K	NIST Webbook
tc	544.45	K	Joback Method
tf	148.50 ± 0.50	K	NIST Webbook
tf	147.40 ± 0.50	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.52	J/mol×K	366.30	Joback Method
cpg	191.02	J/mol×K	395.99	Joback Method
cpg	203.85	J/mol×K	425.68	Joback Method
cpg	216.06	J/mol×K	455.38	Joback Method
cpg	227.66	J/mol×K	485.07	Joback Method
cpg	238.68	J/mol×K	514.76	Joback Method
cpg	249.15	J/mol×K	544.45	Joback Method
dvisc	0.0010653	Pa×s	186.59	Joback Method
dvisc	0.0007611	Pa×s	216.54	Joback Method
dvisc	0.0005900	Pa×s	246.49	Joback Method
dvisc	0.0004833	Pa×s	276.44	Joback Method
dvisc	0.0004117	Pa×s	306.40	Joback Method
dvisc	0.0003608	Pa×s	336.35	Joback Method
dvisc	0.0003231	Pa×s	366.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930574&Units=SI
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

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
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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