

sec-Butylcyclopropane

Other names:	Cyclopropane, sec-butyl- sec-Butylcyclopropane
Inchi:	InChI=1S/C7H14/c1-3-6(2)7-4-5-7/h6-7H,3-5H2,1-2H3
InchiKey:	INSSHDIMRIMVLZ-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCC(C)C1CC1
Mol. weight [g/mol]:	98.19

Physical Properties

Property code	Value	Unit	Source
af	0.2931		Cheméo Relay (1.0)
chl	-4372.00	kJ/mol	NIST Webbook
hfus	8.50	kJ/mol	Joback Method
ie	9.12	eV	Cheméo Relay (1.0)
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	364.13 ± 0.10	K	NIST Webbook
tb	364.13 ± 0.10	K	NIST Webbook
tc	559.46	K	Cheméo Relay (1.0)
tf	151.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.35	J/mol×K	365.86	Joback Method
cpg	251.00	J/mol×K	548.36	Joback Method
cpg	240.28	J/mol×K	517.94	Joback Method
cpg	228.97	J/mol×K	487.53	Joback Method
cpg	217.06	J/mol×K	457.11	Joback Method
cpg	204.50	J/mol×K	426.69	Joback Method
cpg	191.27	J/mol×K	396.28	Joback Method
dvisc	0.0005101	Pa×s	268.73	Joback Method
dvisc	0.0003139	Pa×s	365.86	Joback Method

dvisc	0.0003576	Pa×s	333.48	Joback Method
dvisc	0.0004190	Pa×s	301.10	Joback Method
dvisc	0.0014366	Pa×s	171.59	Joback Method
dvisc	0.0006553	Pa×s	236.35	Joback Method
dvisc	0.0009117	Pa×s	203.97	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5750027&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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

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