Butane, 1-chloro-2-methyl-, (S)-

Inchi: InChI=1S/C5H11Cl/c1-3-5(2)4-6/h5H,3-4H2,1-2H3/t5-/m1/s1
InchiKey: IWAKWOFEHSYKSI-RXMQYKEDSA-N
Formula: C5H11Cl
SMILES: CCC(C)CCl
Mol. weight [g/mol]: 106.59
CAS: 40560-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.15	kJ/mol	Joback Method
hf	-167.55	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	30.72	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	2.271		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	372.70 ± 3.00	K	NIST Webbook
tb	372.65 ± 1.00	K	NIST Webbook
tc	527.49	K	Joback Method
tf	161.03	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.99	J/mol×K	350.79	Joback Method
cpg	193.96	J/mol×K	498.04	Joback Method
cpg	186.05	J/mol×K	468.59	Joback Method
cpg	177.80	J/mol×K	439.14	Joback Method
cpg	169.22	J/mol×K	409.69	Joback Method
cpg	160.28	J/mol×K	380.24	Joback Method
cpg	201.54	J/mol×K	527.49	Joback Method
dvisc	0.0002823	Pa×s	350.79	Joback Method

dvisc	0.0003734	Pa×s	319.16	Joback Method
dvisc	0.0005253	Pa×s	287.54	Joback Method
dvisc	0.0008040	Pa×s	255.91	Joback Method
dvisc	0.0013876	Pa×s	224.28	Joback Method
dvisc	0.0028647	Pa×s	192.66	Joback Method
dvisc	0.0078623	Pa×s	161.03	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=C40560290&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