

Sec-C4H9Cl

Inchi: InChI=1S/C4H9Cl/c1-3-4(2)5/h4H,3H2,1-2H3
InchiKey: BSPCSKHALVHRSR-UHFFFAOYSA-N
Formula: C4H9Cl
SMILES: CCC(C)Cl
Mol. weight [g/mol]: 92.57
CAS: 53178-20-4

Physical Properties

Property code	Value	Unit	Source
chl	-2691.10 ± 8.40	kJ/mol	NIST Webbook
gf	-31.57	kJ/mol	Joback Method
hf	-146.91	kJ/mol	Joback Method
hfus	6.79	kJ/mol	Joback Method
hvap	31.56 ± 0.06	kJ/mol	NIST Webbook
log10ws	-1.76		Crippen Method
logp	2.024		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	341.40	K	NIST Webbook
tc	504.53	K	Joback Method
tf	149.76	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.70	J/mol×K	327.91	Joback Method
cpg	126.45	J/mol×K	357.35	Joback Method
cpg	133.91	J/mol×K	386.78	Joback Method
cpg	141.08	J/mol×K	416.22	Joback Method
cpg	147.98	J/mol×K	445.66	Joback Method
cpg	154.60	J/mol×K	475.09	Joback Method
cpg	160.95	J/mol×K	504.53	Joback Method
dvisc	0.0070575	Pa×s	149.76	Joback Method

dvisc	0.0026220	Pa×s	179.45	Joback Method
dvisc	0.0012903	Pa×s	209.14	Joback Method
dvisc	0.0007574	Pa×s	238.83	Joback Method
dvisc	0.0005002	Pa×s	268.53	Joback Method
dvisc	0.0003588	Pa×s	298.22	Joback Method
dvisc	0.0002733	Pa×s	327.91	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=C53178204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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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