2-Pentanol, 3-chloro-4-methyl-, (R*,S*)-(.+/-.)-

Other names: 2-Pentanol, 3-chloro-4-methyl-, (R*,S*)-(±)-
3-Chloro-4-methyl-2-pentanol
Inchi: InChI=1S/C6H13ClO/c1-4(2)6(7)5(3)8/h4-6,8H,1-3H3
InchiKey: MWICNGBDJPEOGW-UHFFFAOYSA-N
Formula: C6H13ClO
SMILES: CC(C)C(Cl)C(C)O
Mol. weight [g/mol]: 136.62
CAS: 74685-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-156.43	kJ/mol	Joback Method
hf	-350.98	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.631		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
ripol	1689.00		NIST Webbook
tb	464.97	K	Joback Method
tc	643.18	K	Joback Method
tf	203.12	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.91	J/mol×K	464.97	Joback Method
cpg	243.94	J/mol×K	494.67	Joback Method
cpg	253.52	J/mol×K	524.37	Joback Method
cpg	262.69	J/mol×K	554.07	Joback Method
cpg	271.44	J/mol×K	583.78	Joback Method
cpg	279.79	J/mol×K	613.48	Joback Method

cpg	287.75	J/mol×K	643.18	Joback Method
dvisc	0.5632094	Pa×s	203.12	Joback Method
dvisc	0.0458888	Pa×s	246.76	Joback Method
dvisc	0.0079440	Pa×s	290.40	Joback Method
dvisc	0.0021747	Pa×s	334.05	Joback Method
dvisc	0.0008031	Pa×s	377.69	Joback Method
dvisc	0.0003646	Pa×s	421.33	Joback Method
dvisc	0.0001919	Pa×s	464.97	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=C74685486&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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