3,5-Dichlorobenzyl alcohol

Other names: 3,5-Dichlorobenzyl alcohol
Inchi: InChI=1S/C7H6Cl2O/c8-6-1-5(4-10)2-7(9)3-6/h1-3,10H,4H2
InchiKey: VSNNLLQKDRCKCB-UHFFFAOYSA-N
Formula: C7H6Cl2O
SMILES: OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 177.03

Physical Properties

Property code	Value	Unit	Source
hf	-169.40	kJ/mol	Cheméo Relay (1.0)
hfus	19.63	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-2.27		Cheméo Relay (1.0)
logp	2.486		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
tb	512.11	K	Cheméo Relay (1.0)
tf	321.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.64	J/mol×K	563.24	Joback Method
cpg	232.32	J/mol×K	598.63	Joback Method
cpg	239.53	J/mol×K	634.02	Joback Method
cpg	246.28	J/mol×K	669.42	Joback Method
cpg	252.60	J/mol×K	704.81	Joback Method
cpg	258.50	J/mol×K	740.20	Joback Method
cpg	264.01	J/mol×K	775.59	Joback Method
dvisc	0.0037516	Pa×s	340.77	Joback Method
dvisc	0.0015984	Pa×s	377.85	Joback Method
dvisc	0.0007932	Pa×s	414.93	Joback Method
dvisc	0.0004416	Pa×s	452.00	Joback Method
dvisc	0.0002687	Pa×s	489.08	Joback Method

dvisc	0.0001753	Pa×s	526.16	Joback Method
dvisc	0.0001210	Pa×s	563.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C60211576&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point