2,6-dichlorobenzyl alcohol

Other names: (2,6-dichlorophenyl)methanol
Inchi: InChI=1S/C7H6Cl2O/c8-6-2-1-3-7(9)5(6)4-10/h1-3,10H,4H2
InchiKey: WKKHCCZLKYKUDN-UHFFFAOYSA-N
Formula: C7H6Cl2O
SMILES: OCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 177.03
CAS: 15258-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-59.47	kJ/mol	Joback Method
hf	-157.93	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-2.10		Aqueous Solubility Prediction Method
logp	2.486		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	563.24	K	Joback Method
tc	775.59	K	Joback Method
tf	370.65	K	Aqueous Solubility Prediction Method
vc	0.436	m3/kmol	Joback Method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15258738&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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