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

Physical Properties

Property code	Value	Unit	Source
af	0.5997		Cheméo Relay (1.0)
gf	-59.47	kJ/mol	Joback Method
hf	-175.02	kJ/mol	Cheméo Relay (1.0)
hfus	19.63	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
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	536.27	K	Cheméo Relay (1.0)
tc	790.64	K	Cheméo Relay (1.0)
tf	370.65	K	Aqueous Solubility Prediction Method
vc	0.404	m3/kmol	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	264.01	J/mol×K	775.59	Joback Method
cpg	258.50	J/mol×K	740.20	Joback Method
cpg	252.60	J/mol×K	704.81	Joback Method
cpg	246.28	J/mol×K	669.42	Joback Method

cpg	239.53	J/mol×K	634.02	Joback Method
cpg	232.32	J/mol×K	598.63	Joback Method
dvisc	0.0004416	Pa×s	452.00	Joback Method
dvisc	0.0001210	Pa×s	563.24	Joback Method
dvisc	0.0001753	Pa×s	526.16	Joback Method
dvisc	0.0002687	Pa×s	489.08	Joback Method
dvisc	0.0037516	Pa×s	340.77	Joback Method
dvisc	0.0007932	Pa×s	414.93	Joback Method
dvisc	0.0015984	Pa×s	377.85	Joback Method

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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

Legend

af: Acentric Factor

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

ie: Ionization energy

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