2,5-Dichlorophenyl methyl carbinol

Other names: 2,5-Dichlorophenylmethylcarbinol
Benzenemethanol, 2,5-dichloro-«alpha»-methyl-
2,5-Dichloro-alpha-methylbenzyl alcohol
Inchi: InChI=1S/C8H8Cl2O/c1-5(11)7-4-6(9)2-3-8(7)10/h2-5,11H,1H3
InchiKey: RDMKUSDLLGKMCK-UHFFFAOYSA-N
Formula: C8H8Cl2O
SMILES: CC(O)c1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 191.06

Physical Properties

Property code	Value	Unit	Source
hf	-227.49	kJ/mol	Cheméo Relay (1.0)
hfus	18.70	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Cheméo Relay (1.0)
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-2.22		Cheméo Relay (1.0)
logp	3.047		Crippen Method
mcvol	130.170	ml/mol	McGowan Method
tb	519.71	K	Cheméo Relay (1.0)
tf	343.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.61	J/mol×K	585.68	Joback Method
cpg	277.58	J/mol×K	621.23	Joback Method
cpg	285.99	J/mol×K	656.77	Joback Method
cpg	293.87	J/mol×K	692.32	Joback Method
cpg	301.24	J/mol×K	727.87	Joback Method
cpg	308.12	J/mol×K	763.41	Joback Method
cpg	314.53	J/mol×K	798.96	Joback Method
dvisc	0.0047267	Pa×s	337.04	Joback Method
dvisc	0.0017296	Pa×s	378.48	Joback Method
dvisc	0.0007718	Pa×s	419.92	Joback Method

dvisc	0.0003981	Pa×s	461.36	Joback Method
dvisc	0.0002291	Pa×s	502.80	Joback Method
dvisc	0.0001434	Pa×s	544.24	Joback Method
dvisc	0.0000959	Pa×s	585.68	Joback Method

Sources

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=C1475123&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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