3,5-Dichlorobenzyl alcohol, acetate

Inchi: InChI=1S/C9H8Cl2O2/c1-6(12)13-5-7-2-8(10)4-9(11)3-7/h2-4H,5H2,1H3
InchiKey: AUBLCENCKCEUKL-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: CC(=O)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 219.07

Physical Properties

Property code	Value	Unit	Source
hfus	23.51	kJ/mol	Joback Method
hvap	70.32	kJ/mol	Cheméo Relay (1.0)
logp	3.056		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	524.93	K	Cheméo Relay (1.0)
tf	288.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.99	J/mol×K	593.11	Joback Method
cpg	313.48	J/mol×K	630.97	Joback Method
cpg	323.31	J/mol×K	668.84	Joback Method
cpg	332.51	J/mol×K	706.70	Joback Method
cpg	341.08	J/mol×K	744.56	Joback Method
cpg	349.03	J/mol×K	782.43	Joback Method
cpg	356.37	J/mol×K	820.29	Joback Method
dvisc	0.0012799	Pa×s	374.65	Joback Method
dvisc	0.0008364	Pa×s	411.06	Joback Method
dvisc	0.0005857	Pa×s	447.47	Joback Method
dvisc	0.0004328	Pa×s	483.88	Joback Method
dvisc	0.0003336	Pa×s	520.29	Joback Method
dvisc	0.0002661	Pa×s	556.70	Joback Method
dvisc	0.0002182	Pa×s	593.11	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=C85263043&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point