Acetic acid, (2,4-dichlorophenyl)methyl ester

Inchi: InChI=1S/C9H8Cl2O2/c1-6(12)13-5-7-2-3-8(10)4-9(7)11/h2-4H,5H2,1H3
InchiKey: TXJMBLACZHJNAE-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: CC(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 219.06

Physical Properties

Property code	Value	Unit	Source
gf	-139.73	kJ/mol	Joback Method
hf	-291.78	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.056		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1515.00		NIST Webbook
tb	593.11	K	Joback Method
tc	820.29	K	Joback Method
tf	374.65	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.99	J/mol×K	593.11	Joback Method
cpg	349.03	J/mol×K	782.43	Joback Method
cpg	341.08	J/mol×K	744.56	Joback Method
cpg	332.51	J/mol×K	706.70	Joback Method
cpg	323.31	J/mol×K	668.84	Joback Method
cpg	313.48	J/mol×K	630.97	Joback Method
cpg	356.37	J/mol×K	820.29	Joback Method
dvisc	0.0002182	Pa×s	593.11	Joback Method
dvisc	0.0002661	Pa×s	556.70	Joback Method

dvisc	0.0003336	Pa×s	520.29	Joback Method
dvisc	0.0004328	Pa×s	483.88	Joback Method
dvisc	0.0005857	Pa×s	447.47	Joback Method
dvisc	0.0008364	Pa×s	411.06	Joback Method
dvisc	0.0012799	Pa×s	374.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368902&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume