Dichloroacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C10H10Cl2O2/c1-6-3-7(2)5-8(4-6)14-10(13)9(11)12/h3-5,9H,1-2H3
InchiKey: NGJFMOALFGIQLY-UHFFFAOYSA-N
Formula: C10H10Cl2O2
SMILES: Cc1cc(C)cc(OC(=O)C(Cl)Cl)c1
Mol. weight [g/mol]: 233.09

Physical Properties

Property code	Value	Unit	Source
gf	-133.75	kJ/mol	Joback Method
hf	-317.70	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.013		Crippen Method
mcvol	159.920	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	615.55	K	Joback Method
tc	843.20	K	Joback Method
tf	370.92	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.65	J/mol×K	615.55	Joback Method
cpg	400.81	J/mol×K	805.26	Joback Method
cpg	392.02	J/mol×K	767.32	Joback Method
cpg	382.52	J/mol×K	729.37	Joback Method
cpg	372.30	J/mol×K	691.43	Joback Method
cpg	361.35	J/mol×K	653.49	Joback Method
cpg	408.90	J/mol×K	843.20	Joback Method
dvisc	0.0001846	Pa×s	615.55	Joback Method

dvisc	0.0002306	Pa×s	574.78	Joback Method
dvisc	0.0002981	Pa×s	534.01	Joback Method
dvisc	0.0004019	Pa×s	493.24	Joback Method
dvisc	0.0005720	Pa×s	452.46	Joback Method
dvisc	0.0008731	Pa×s	411.69	Joback Method
dvisc	0.0014623	Pa×s	370.92	Joback Method

Sources

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=U307585&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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