2-Chloropropionic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C9H8Cl2O2/c1-6(10)9(12)13-8-4-2-7(11)3-5-8/h2-6H,1H3
InchiKey: ZTFHVLFFQQCYQH-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: CC(Cl)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 219.06

Physical Properties

Property code	Value	Unit	Source
gf	-132.54	kJ/mol	Joback Method
hf	-285.59	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.873		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	587.69	K	Joback Method
tc	818.84	K	Joback Method
tf	347.13	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.59	J/mol×K	587.69	Joback Method
cpg	315.62	J/mol×K	626.22	Joback Method
cpg	325.90	J/mol×K	664.74	Joback Method
cpg	335.46	J/mol×K	703.27	Joback Method
cpg	344.32	J/mol×K	741.79	Joback Method
cpg	352.48	J/mol×K	780.32	Joback Method

cpg	359.97	J/mol×K	818.84	Joback Method
dvisc	0.0019276	Pa×s	347.13	Joback Method
dvisc	0.0010973	Pa×s	387.22	Joback Method
dvisc	0.0006944	Pa×s	427.32	Joback Method
dvisc	0.0004752	Pa×s	467.41	Joback Method
dvisc	0.0003454	Pa×s	507.50	Joback Method
dvisc	0.0002630	Pa×s	547.60	Joback Method
dvisc	0.0002078	Pa×s	587.69	Joback Method

Sources

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=U357777&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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