

2-Chloropropionic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C10H11ClO3/c1-7(11)10(12)14-9-5-3-8(13-2)4-6-9/h3-7H,1-2H3
InchiKey:	LHPTYGDRPPSKNI-UHFFFAOYSA-N
Formula:	C10H11ClO3
SMILES:	COc1ccc(OC(=O)C(C)Cl)cc1
Mol. weight [g/mol]:	214.65

Physical Properties

Property code	Value	Unit	Source
gf	-217.19	kJ/mol	Joback Method
hf	-422.71	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.228		Crippen Method
mvol	153.550	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	595.56	K	Joback Method
tc	815.68	K	Joback Method
tf	350.71	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.85	J/molxK	595.56	Joback Method
cpg	362.46	J/molxK	632.25	Joback Method
cpg	374.34	J/molxK	668.93	Joback Method
cpg	385.49	J/molxK	705.62	Joback Method
cpg	395.91	J/molxK	742.31	Joback Method
cpg	405.60	J/molxK	779.00	Joback Method
cpg	414.56	J/molxK	815.68	Joback Method
dvisc	0.0015181	Paxs	350.71	Joback Method

dvisc	0.0008545	Paxs	391.52	Joback Method
dvisc	0.0005361	Paxs	432.33	Joback Method
dvisc	0.0003645	Paxs	473.13	Joback Method
dvisc	0.0002635	Paxs	513.94	Joback Method
dvisc	0.0001998	Paxs	554.75	Joback Method
dvisc	0.0001573	Paxs	595.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U307754&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

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