

Cyclopropanecarboxylic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C10H9ClO2/c11-8-3-5-9(6-4-8)13-10(12)7-1-2-7/h3-7H,1-2H2
InchiKey:	VDWGAQSMDCDWER-UHFFFAOYSA-N
Formula:	C10H9ClO2
SMILES:	O=C(Oc1ccc(Cl)cc1)C1CC1
Mol. weight [g/mol]:	196.63

Physical Properties

Property code	Value	Unit	Source
gf	-49.00	kJ/mol	Joback Method
hf	-212.41	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.655		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	580.32	K	Joback Method
tc	814.95	K	Joback Method
tf	361.42	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.89	J/mol×K	580.32	Joback Method
cpg	323.91	J/mol×K	619.43	Joback Method
cpg	335.97	J/mol×K	658.53	Joback Method
cpg	347.14	J/mol×K	697.64	Joback Method
cpg	357.46	J/mol×K	736.74	Joback Method
cpg	367.00	J/mol×K	775.85	Joback Method
cpg	375.80	J/mol×K	814.95	Joback Method
dvisc	0.0018016	Paxs	361.42	Joback Method

dvisc	0.0013094	Paxs	397.90	Joback Method
dvisc	0.0010040	Paxs	434.39	Joback Method
dvisc	0.0008022	Paxs	470.87	Joback Method
dvisc	0.0006620	Paxs	507.35	Joback Method
dvisc	0.0005606	Paxs	543.84	Joback Method
dvisc	0.0004847	Paxs	580.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307522&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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