

4-Chlorobutyric acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C10H10Cl2O2/c11-7-1-2-10(13)14-9-5-3-8(12)4-6-9/h3-6H,1-2,7H2
InchiKey:	BZXFHJFAMAYMNE-UHFFFAOYSA-N
Formula:	C10H10Cl2O2
SMILES:	O=C(CCCCl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	233.09

Physical Properties

Property code	Value	Unit	Source
gf	-121.68	kJ/mol	Joback Method
hf	-300.95	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.264		Crippen Method
mcvol	159.920	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1652.00		NIST Webbook
tb	611.01	K	Joback Method
tc	832.99	K	Joback Method
tf	373.40	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.27	J/mol×K	611.01	Joback Method
cpg	361.90	J/mol×K	648.01	Joback Method
cpg	372.77	J/mol×K	685.00	Joback Method
cpg	382.92	J/mol×K	722.00	Joback Method
cpg	392.36	J/mol×K	759.00	Joback Method
cpg	401.10	J/mol×K	795.99	Joback Method
cpg	409.17	J/mol×K	832.99	Joback Method
dvisc	0.0015241	Pa×s	373.40	Joback Method
dvisc	0.0009249	Pa×s	413.00	Joback Method

dvisc	0.0006125	Pa×s	452.60	Joback Method
dvisc	0.0004335	Pa×s	492.21	Joback Method
dvisc	0.0003230	Pa×s	531.81	Joback Method
dvisc	0.0002506	Pa×s	571.41	Joback Method
dvisc	0.0002010	Pa×s	611.01	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=U307601&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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