

4-Chlorobutyric acid, 3,4-dimethylphenyl ester

Inchi:	InChI=1S/C12H15ClO2/c1-9-5-6-11(8-10(9)2)15-12(14)4-3-7-13/h5-6,8H,3-4,7H2,1-2H3
InchiKey:	FRQFOERERRZLDX-UHFFFAOYSA-N
Formula:	C12H15ClO2
SMILES:	Cc1ccc(OC(=O)CCCCl)cc1C
Mol. weight [g/mol]:	226.70

Physical Properties

Property code	Value	Unit	Source
gf	-102.54	kJ/mol	Joback Method
hf	-337.96	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.228		Crippen Method
mvol	175.860	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		NIST Webbook
tb	624.32	K	Joback Method
tc	836.12	K	Joback Method
tf	378.54	K	Joback Method
vc	0.672	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.60	J/molxK	624.32	Joback Method
cpg	434.41	J/molxK	659.62	Joback Method
cpg	447.44	J/molxK	694.92	Joback Method
cpg	459.71	J/molxK	730.22	Joback Method
cpg	471.22	J/molxK	765.52	Joback Method
cpg	481.99	J/molxK	800.82	Joback Method
cpg	492.04	J/molxK	836.12	Joback Method
dvisc	0.0012490	Paxs	378.54	Joback Method

dvisc	0.0007630	Paxs	419.50	Joback Method
dvisc	0.0005088	Paxs	460.47	Joback Method
dvisc	0.0003625	Paxs	501.43	Joback Method
dvisc	0.0002718	Paxs	542.39	Joback Method
dvisc	0.0002123	Paxs	583.36	Joback Method
dvisc	0.0001712	Paxs	624.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357387&Units=SI
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

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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