

4-Chlorobutyric acid, 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C10H9Cl3O2/c11-6-2-5-9(14)15-8-4-1-3-7(12)10(8)13/h1,3-4H,2,5-6H2
InchiKey:	GKKJTDZZCWNXHN-UHFFFAOYSA-N
Formula:	C10H9Cl3O2
SMILES:	O=C(CCCCl)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	267.54

Physical Properties

Property code	Value	Unit	Source
gf	-143.24	kJ/mol	Joback Method
hf	-328.16	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.918		Crippen Method
mvol	172.160	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1896.00		NIST Webbook
tb	653.42	K	Joback Method
tc	879.65	K	Joback Method
tf	415.84	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.77	J/molxK	653.42	Joback Method
cpg	417.42	J/molxK	841.94	Joback Method
cpg	409.66	J/molxK	804.24	Joback Method
cpg	401.23	J/molxK	766.53	Joback Method
cpg	392.12	J/molxK	728.83	Joback Method
cpg	382.30	J/molxK	691.12	Joback Method
cpg	424.52	J/molxK	879.65	Joback Method
dvisc	0.0001846	Paxs	653.42	Joback Method
dvisc	0.0002264	Paxs	613.82	Joback Method

dvisc	0.0002855	Paxs	574.23	Joback Method
dvisc	0.0003726	Paxs	534.63	Joback Method
dvisc	0.0005075	Paxs	495.03	Joback Method
dvisc	0.0007294	Paxs	455.44	Joback Method
dvisc	0.0011233	Paxs	415.84	Joback Method

Sources

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=U357389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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