4-Chlorobutyric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C10H9Cl3O2/c11-5-1-2-10(14)15-7-3-4-8(12)9(13)6-7/h3-4,6H,1-2,5H2
InchiKey: DILXPIIEMXUPCA-UHFFFAOYSA-N
Formula: C10H9Cl3O2
SMILES: O=C(CCCCl)Oc1ccc(Cl)c(Cl)c1
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
mcvol	172.160	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	653.42	K	Joback Method
tc	879.65	K	Joback Method
tf	415.84	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.77	J/mol×K	653.42	Joback Method
cpg	417.42	J/mol×K	841.94	Joback Method
cpg	409.66	J/mol×K	804.24	Joback Method
cpg	401.23	J/mol×K	766.53	Joback Method
cpg	392.12	J/mol×K	728.83	Joback Method
cpg	382.30	J/mol×K	691.12	Joback Method
cpg	424.52	J/mol×K	879.65	Joback Method

dvisc	0.0001846	Pa×s	653.42	Joback Method
dvisc	0.0002264	Pa×s	613.82	Joback Method
dvisc	0.0002855	Pa×s	574.23	Joback Method
dvisc	0.0003726	Pa×s	534.63	Joback Method
dvisc	0.0005075	Pa×s	495.03	Joback Method
dvisc	0.0007294	Pa×s	455.44	Joback Method
dvisc	0.0011233	Pa×s	415.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357773&Units=SI
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

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