

4-Chlorobutyric acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C10H8Cl4O2/c11-3-1-2-10(15)16-9-5-7(13)6(12)4-8(9)14/h4-5H,1-3H2
InchiKey:	XMAYIRLGYAMNQD-UHFFFAOYSA-N
Formula:	C10H8Cl4O2
SMILES:	O=C(CCCCl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	301.98

Physical Properties

Property code	Value	Unit	Source
gf	-164.80	kJ/mol	Joback Method
hf	-355.37	kJ/mol	Joback Method
hfus	34.10	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.571		Crippen Method
mcvol	184.400	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinsol	2023.00		NIST Webbook
tb	695.83	K	Joback Method
tc	925.83	K	Joback Method
tf	458.28	K	Joback Method
vc	0.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.31	J/molxK	695.83	Joback Method
cpg	431.96	J/molxK	887.49	Joback Method
cpg	425.16	J/molxK	849.16	Joback Method
cpg	417.71	J/molxK	810.83	Joback Method
cpg	409.59	J/molxK	772.50	Joback Method
cpg	400.80	J/molxK	734.16	Joback Method
cpg	438.10	J/molxK	925.83	Joback Method
dvisc	0.0001672	Paxs	695.83	Joback Method
dvisc	0.0002021	Paxs	656.24	Joback Method

dvisc	0.0002503	Paxs	616.65	Joback Method
dvisc	0.0003192	Paxs	577.06	Joback Method
dvisc	0.0004219	Paxs	537.46	Joback Method
dvisc	0.0005829	Paxs	497.87	Joback Method
dvisc	0.0008517	Paxs	458.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360645&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

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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