Butanoic acid, 4-(2,4,5-trichlorophenoxy)-

Other names:	Butyric acid, 4-(2,4,5-trichlorophenoxy)-
	«gamma»-(2,4,5-Trichlorophenoxy)butyric acid
	2,4,5-TB
	4-(2,4,5-Trichlorophenoxy)Butyric acid
	2,4,5-T Butyric acid
	4-(2,4,5-Trichlorophenoxy)butanoic acid
Inchi:	InChI=1S/C10H9Cl3O3/c11-6-4-8(13)9(5-7(6)12)16-3-1-2-10(14)15/h4-5H,1-3H2,(H,14,1
InchiKey:	RTWCZQFXFMXXKP-UHFFFAOYSA-N
Formula:	C10H9Cl3O3
SMILES:	O=C(O)CCCOc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	283.54
CAS:	93-80-1

Physical Properties

Property code	Value	Unit	Source
gf	-289.69	kJ/mol	Joback Method
hf	-491.86	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.890		Crippen Method
mcvol	178.030	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	750.58	K	Joback Method
tc	962.26	K	Joback Method
tf	386.80 ± 0.20	K	NIST Webbook
tf	388.10 ± 0.20	K	NIST Webbook
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.17	J/mol×K	750.58	Joback Method
cpg	420.49	J/mol×K	785.86	Joback Method

cpg	428.22	J/mol×K	821.14	Joback Method
cpg	435.36	J/mol×K	856.42	Joback Method
cpg	441.93	J/mol×K	891.70	Joback Method
cpg	447.93	J/mol×K	926.98	Joback Method
cpg	453.38	J/mol×K	962.26	Joback Method
dvisc	0.0005473	Pa×s	489.18	Joback Method
dvisc	0.0002932	Pa×s	532.75	Joback Method
dvisc	0.0001726	Pa×s	576.31	Joback Method
dvisc	0.0001095	Pa×s	619.88	Joback Method
dvisc	0.0000737	Pa×s	663.45	Joback Method
dvisc	0.0000521	Pa×s	707.01	Joback Method
dvisc	0.0000384	Pa×s	750.58	Joback Method
hfust	30.28	kJ/mol	386.70	NIST Webbook

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=C93801&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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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