2-(p-Chlorophenoxy)-2-methylpropionic acid

Other names:	(p-Chlorophenoxy)isobutyric acid
	2-(4-Chlorophenoxy)-2-methylpropanoic acid
	2-(4-Chlorophenoxy)-2-methylpropionic acid
	2-(p-Chlorophenoxy)-2-methylpropanoic acid
	2-(p-Chlorophenoxy)-2-methylpropionic acid
	2-(p-Chlorophenoxy)isobutyric acid
	4-(Chlorophenoxy)isobutyric acid
	4-CPIB
	Acetic acid, (p-chlorophenoxy)dimethyl-
	Acide (p-chlorophenoxy)-2 methyl-2 propionique
	CPIB
	Chlorfibrinic acid
	Chlorofibrinic acid
	Chlorophibrinic acid
	Clofibrate free acid
	Clofibrin
	Clofibrinic acid
	Clofibrinsaeure
	NSC 1149
	PCIB
	PCPIB
	Propanoic acid, 2-(4-chlorophenoxy)-2-methyl-
	Propanoic acid, 2-methyl, 2-(4-chlorophenyloxy)
	Propionic acid, 2-(p-chlorophenoxy)-2-methyl-
	Regadrin
	Regulipid
	«alpha»-(4-Chlorophenoxy)-«alpha»-methylpropionic acid
	«alpha»-(4-Chlorophenoxy)isobutyric acid
	«alpha»-(p-Chlorophenoxy)isobutyric acid
Inchi:	InChI=1S/C10H11ClO3/c1-10(2,9(12)13)14-8-5-3-7(11)4-6-8/h3-6H,1-2H3,(H,12,13)
InchiKey:	TXCGAZHTZHNUAI-UHFFFAOYSA-N
Formula:	C10H11ClO3
SMILES:	CC(C)(Oc1ccc(Cl)cc1)C(=O)O
Mol. weight [g/mol]:	214.65

Physical Properties

Property code	Value	Unit	Source

hf	-526.48	kJ/mol	Cheméo Relay (1.0)
hfus	18.97	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-2.59		Cheméo Relay (1.0)
logp	2.582		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
tb	553.27	K	Cheméo Relay (1.0)
tf	394.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.92	J/mol×K	662.53	Joback Method
cpg	387.37	J/mol×K	698.19	Joback Method
cpg	397.08	J/mol×K	733.85	Joback Method
cpg	406.08	J/mol×K	769.51	Joback Method
cpg	414.40	J/mol×K	805.17	Joback Method
cpg	422.09	J/mol×K	840.82	Joback Method
cpg	429.18	J/mol×K	876.48	Joback Method
dvisc	0.0017046	Pa×s	406.72	Joback Method
dvisc	0.0007134	Pa×s	449.36	Joback Method
dvisc	0.0003472	Pa×s	491.99	Joback Method
dvisc	0.0001896	Pa×s	534.62	Joback Method
dvisc	0.0001132	Pa×s	577.26	Joback Method
dvisc	0.0000725	Pa×s	619.89	Joback Method
dvisc	0.0000492	Pa×s	662.53	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C882097&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point