Propanoic acid, 2-(4-chlorophenoxy)-2-methyl-, methyl ester

Other names: CPIB methyl ester
2-(4-Chlorophenoxy)-2-methylpropanoic acid methyl ester
Propionic acid, 2-(p-chlorophenoxy)-2-methyl-, methyl ester
Clofibrate Me

Inchi: InChI=1S/C11H13ClO3/c1-11(2,10(13)14-3)15-9-6-4-8(12)5-7-9/h4-7H,1-3H3

InchiKey: UXIVINXAZVEIMC-UHFFFAOYSA-N

Formula: C11H13ClO3

SMILES: COC(=O)C(C)(C)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 228.67

CAS: 55162-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-203.49	kJ/mol	Joback Method
hf	-446.82	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.670		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1472.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2025.00		NIST Webbook
tb	615.65	K	Joback Method
tc	840.24	K	Joback Method
tf	379.40	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	400.61	J/mol×K	615.65	Joback Method
cpg	414.32	J/mol×K	653.08	Joback Method
cpg	427.11	J/mol×K	690.51	Joback Method
cpg	439.01	J/mol×K	727.95	Joback Method
cpg	450.04	J/mol×K	765.38	Joback Method
cpg	460.23	J/mol×K	802.81	Joback Method
cpg	469.60	J/mol×K	840.24	Joback Method
dvisc	0.0012806	Pa×s	379.40	Joback Method
dvisc	0.0007368	Pa×s	418.78	Joback Method
dvisc	0.0004661	Pa×s	458.15	Joback Method
dvisc	0.0003171	Pa×s	497.52	Joback Method
dvisc	0.0002282	Pa×s	536.90	Joback Method
dvisc	0.0001718	Pa×s	576.27	Joback Method
dvisc	0.0001342	Pa×s	615.65	Joback Method

Sources

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=C55162419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume