(3-Chloro-4-hexyloxy-phenyl)-acetic acid, methyl ester

Inchi: InChI=1S/C15H21ClO3/c1-3-4-5-6-9-19-14-8-7-12(10-13(14)16)11-15(17)18-2/h7-8,10H,

InchiKey: KXLBCBBKKRMVEX-UHFFFAOYSA-N

Formula: C15H21ClO3

SMILES: CCCCCCOc1ccc(CC(=O)OC)cc1Cl

Mol. weight [g/mol]: 284.78

Physical Properties

Property code	Value	Unit	Source
gf	-182.28	kJ/mol	Joback Method
hf	-532.10	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.015		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2036.40		NIST Webbook
tb	715.38	K	Joback Method
tc	916.91	K	Joback Method
tf	434.58	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.38	J/mol×K	715.38	Joback Method
cpg	617.50	J/mol×K	748.97	Joback Method
cpg	631.73	J/mol×K	782.56	Joback Method
cpg	645.08	J/mol×K	816.14	Joback Method
cpg	657.56	J/mol×K	849.73	Joback Method
cpg	669.17	J/mol×K	883.32	Joback Method
cpg	679.92	J/mol×K	916.91	Joback Method
dvisc	0.0007768	Pa×s	434.58	Joback Method
dvisc	0.0004628	Pa×s	481.38	Joback Method

dvisc	0.0003022	Pa×s	528.18	Joback Method
dvisc	0.0002115	Pa×s	574.98	Joback Method
dvisc	0.0001562	Pa×s	621.78	Joback Method
dvisc	0.0001204	Pa×s	668.58	Joback Method
dvisc	0.0000960	Pa×s	715.38	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=R158006&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume