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

Inchi: InChI=1S/C17H25ClO3/c1-3-4-5-6-7-8-11-21-16-10-9-14(12-15(16)18)13-17(19)20-2/h9-

InchiKey: XWBZHCRZJKWJEU-UHFFFAOYSA-N

Formula: C17H25ClO3

SMILES: CCCCCCCCOc1ccc(CC(=O)OC)cc1Cl

Mol. weight [g/mol]: 312.83

Physical Properties

Property code	Value	Unit	Source
gf	-165.44	kJ/mol	Joback Method
hf	-573.38	kJ/mol	Joback Method
hfus	41.22	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.795		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2233.40		NIST Webbook
rinpol	2233.40		NIST Webbook
tb	761.14	K	Joback Method
tc	959.53	K	Joback Method
tf	457.12	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.02	J/mol×K	761.14	Joback Method
cpg	728.84	J/mol×K	794.20	Joback Method
cpg	743.69	J/mol×K	827.27	Joback Method
cpg	757.59	J/mol×K	860.33	Joback Method
cpg	770.54	J/mol×K	893.40	Joback Method
cpg	782.57	J/mol×K	926.46	Joback Method
cpg	793.69	J/mol×K	959.53	Joback Method
dvisc	0.0006654	Pa×s	457.12	Joback Method

dvisc	0.0003852	Pa×s	507.79	Joback Method
dvisc	0.0002463	Pa×s	558.46	Joback Method
dvisc	0.0001696	Pa×s	609.13	Joback Method
dvisc	0.0001237	Pa×s	659.80	Joback Method
dvisc	0.0000944	Pa×s	710.47	Joback Method
dvisc	0.0000746	Pa×s	761.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R158011&Units=SI

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