4-(Octyloxy)-3-chlorophenylacetic acid

Inchi: InChI=1S/C16H23ClO3/c1-2-3-4-5-6-7-10-20-15-9-8-13(11-14(15)17)12-16(18)19/h8-9,1
InchiKey: IHBVRZFITXXSHI-UHFFFAOYSA-N
Formula: C16H23ClO3
SMILES: CCCCCCCCOc1ccc(CC(=O)O)cc1Cl
Mol. weight [g/mol]: 298.81

Physical Properties

Property code	Value	Unit	Source
gf	-205.68	kJ/mol	Joback Method
hf	-572.75	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.706		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	808.02	K	Joback Method
tc	1004.20	K	Joback Method
tf	484.44	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.62	J/mol×K	808.02	Joback Method
cpg	701.81	J/mol×K	840.72	Joback Method
cpg	714.17	J/mol×K	873.41	Joback Method
cpg	725.73	J/mol×K	906.11	Joback Method
cpg	736.50	J/mol×K	938.81	Joback Method
cpg	746.51	J/mol×K	971.50	Joback Method
cpg	755.79	J/mol×K	1004.20	Joback Method
dvisc	0.0005429	Pa×s	484.44	Joback Method

dvisc	0.0002371	Pa×s	538.37	Joback Method
dvisc	0.0001204	Pa×s	592.30	Joback Method
dvisc	0.0000684	Pa×s	646.23	Joback Method
dvisc	0.0000425	Pa×s	700.16	Joback Method
dvisc	0.0000282	Pa×s	754.09	Joback Method
dvisc	0.0000198	Pa×s	808.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R31739&Units=SI
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

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