(4-Hexyloxy-phenyl)-acetic acid, methyl ester

Inchi: InChI=1S/C15H22O3/c1-3-4-5-6-11-18-14-9-7-13(8-10-14)12-15(16)17-2/h7-10H,3-6,11-
InchiKey: IUUJCAOZWVHINB-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CCCCCCOc1ccc(CC(=O)OC)cc1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-160.72	kJ/mol	Joback Method
hf	-504.89	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.361		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1874.20		NIST Webbook
tb	672.97	K	Joback Method
tc	869.94	K	Joback Method
tf	392.14	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.00	J/mol×K	672.97	Joback Method
cpg	590.26	J/mol×K	705.80	Joback Method
cpg	605.64	J/mol×K	738.63	Joback Method
cpg	620.13	J/mol×K	771.45	Joback Method
cpg	633.77	J/mol×K	804.28	Joback Method
cpg	646.54	J/mol×K	837.11	Joback Method
cpg	658.47	J/mol×K	869.94	Joback Method
dvisc	0.0010931	Pa×s	392.14	Joback Method
dvisc	0.0006017	Pa×s	438.95	Joback Method

dvisc	0.0003716	Pa×s	485.75	Joback Method
dvisc	0.0002498	Pa×s	532.56	Joback Method
dvisc	0.0001790	Pa×s	579.36	Joback Method
dvisc	0.0001349	Pa×s	626.17	Joback Method
dvisc	0.0001057	Pa×s	672.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158086&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

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

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