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

Inchi: InChI=1S/C16H24O4/c1-4-5-6-7-10-20-14-9-8-13(11-15(14)18-2)12-16(17)19-3/h8-9,11H

InchiKey: OUJRFULDFKOKRZ-UHFFFAOYSA-N

Formula: C16H24O4

SMILES: CCCCCCOc1ccc(CC(=O)OC)cc1OC

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-266.93	kJ/mol	Joback Method
hf	-669.22	kJ/mol	Joback Method
hfus	35.62	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.370		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1988.70		NIST Webbook
rinpol	1988.70		NIST Webbook
tb	723.25	K	Joback Method
tc	918.30	K	Joback Method
tf	438.16	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.44	J/mol×K	723.25	Joback Method
cpg	672.63	J/mol×K	755.76	Joback Method
cpg	687.91	J/mol×K	788.27	Joback Method
cpg	702.27	J/mol×K	820.77	Joback Method
cpg	715.70	J/mol×K	853.28	Joback Method
cpg	728.20	J/mol×K	885.79	Joback Method
cpg	739.76	J/mol×K	918.30	Joback Method
dvisc	0.0006064	Pa×s	438.16	Joback Method

dvisc	0.0003580	Pa×s	485.68	Joback Method
dvisc	0.0002322	Pa×s	533.19	Joback Method
dvisc	0.0001616	Pa×s	580.71	Joback Method
dvisc	0.0001188	Pa×s	628.22	Joback Method
dvisc	0.0000913	Pa×s	675.74	Joback Method
dvisc	0.0000725	Pa×s	723.25	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=R158046&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

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