(3-Methoxy-4-hexyloxy-phenyl)-propionic acid, methyl ester

Inchi: InChI=1S/C17H26O4/c1-4-5-6-7-12-21-15-10-8-14(13-16(15)19-2)9-11-17(18)20-3/h8,10

InchiKey: CCPIWFREECSGFF-UHFFFAOYSA-N

Formula: C17H26O4

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

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-258.51	kJ/mol	Joback Method
hf	-689.86	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.760		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2083.80		NIST Webbook
rinpol	2083.80		NIST Webbook
tb	746.13	K	Joback Method
tc	940.06	K	Joback Method
tf	449.43	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.57	J/mol×K	746.13	Joback Method
cpg	729.09	J/mol×K	778.45	Joback Method
cpg	744.65	J/mol×K	810.77	Joback Method
cpg	759.24	J/mol×K	843.10	Joback Method
cpg	772.86	J/mol×K	875.42	Joback Method
cpg	785.51	J/mol×K	907.74	Joback Method
cpg	797.20	J/mol×K	940.06	Joback Method
dvisc	0.0005622	Pa×s	449.43	Joback Method

dvisc	0.0003272	Pa×s	498.88	Joback Method
dvisc	0.0002099	Pa×s	548.33	Joback Method
dvisc	0.0001450	Pa×s	597.78	Joback Method
dvisc	0.0001059	Pa×s	647.23	Joback Method
dvisc	0.0000809	Pa×s	696.68	Joback Method
dvisc	0.0000641	Pa×s	746.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158051&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