3-(3-methoxy-4-hexyloxy-phenyl)-2-methyl-propio
acid, methyl ester

Inchi: InChI=1S/C18H28O4/c1-5-6-7-8-11-22-16-10-9-15(13-17(16)20-3)12-14(2)18(19)21-4/h9
InchiKey: BQEKLEUILOHYIH-UHFFFAOYSA-N
Formula: C18H28O4
SMILES: CCCCCCOc1ccc(CC(C)C(=O)OC)cc1OC
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-252.53	kJ/mol	Joback Method
hf	-715.78	kJ/mol	Joback Method
hfus	37.28	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.006		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	2090.20		NIST Webbook
rinpol	2090.20		NIST Webbook
tb	768.57	K	Joback Method
tc	964.21	K	Joback Method
tf	445.70	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.26	J/mol×K	768.57	Joback Method
cpg	787.28	J/mol×K	801.18	Joback Method
cpg	803.25	J/mol×K	833.78	Joback Method
cpg	818.17	J/mol×K	866.39	Joback Method
cpg	832.05	J/mol×K	899.00	Joback Method
cpg	844.89	J/mol×K	931.61	Joback Method
cpg	856.68	J/mol×K	964.21	Joback Method
dvisc	0.0005942	Pa×s	445.70	Joback Method

dvisc	0.0003180	Pa×s	499.51	Joback Method
dvisc	0.0001922	Pa×s	553.32	Joback Method
dvisc	0.0001270	Pa×s	607.13	Joback Method
dvisc	0.0000898	Pa×s	660.95	Joback Method
dvisc	0.0000669	Pa×s	714.76	Joback Method
dvisc	0.0000519	Pa×s	768.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157890&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