3-(4-Hydroxy-3-methoxyphenyl)-2-oxopropyl benzoate

Inchi: InChI=1S/C17H16O5/c1-21-16-10-12(7-8-15(16)19)9-14(18)11-22-17(20)13-5-3-2-4-6-13

InchiKey: CEBLIPZJHBZGKI-UHFFFAOYSA-N

Formula: C17H16O5

SMILES: COc1cc(CC(=O)COC(=O)c2ccccc2)ccc1O

Mol. weight [g/mol]: 300.31

CAS: 934248-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-315.01	kJ/mol	Joback Method
hf	-599.53	kJ/mol	Joback Method
hfus	38.84	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.369		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	2537.30		NIST Webbook
rinpol	2537.30		NIST Webbook
tb	879.90	K	Joback Method
tc	1118.81	K	Joback Method
tf	602.75	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.49	J/mol×K	879.90	Joback Method
cpg	712.58	J/mol×K	1078.99	Joback Method
cpg	703.40	J/mol×K	1039.17	Joback Method
cpg	693.58	J/mol×K	999.36	Joback Method
cpg	683.04	J/mol×K	959.54	Joback Method
cpg	671.71	J/mol×K	919.72	Joback Method
cpg	721.22	J/mol×K	1118.81	Joback Method

dvisc	0.0000038	Pa×s	879.90	Joback Method
dvisc	0.0000052	Pa×s	833.71	Joback Method
dvisc	0.0000075	Pa×s	787.52	Joback Method
dvisc	0.0000114	Pa×s	741.33	Joback Method
dvisc	0.0000181	Pa×s	695.13	Joback Method
dvisc	0.0000307	Pa×s	648.94	Joback Method
dvisc	0.0000565	Pa×s	602.75	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=C934248676&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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