

Propanoic acid, 3-hydroxy-3-(3-methoxyphenyl), methyl ester

Inchi:	InChI=1S/C11H14O4/c1-14-9-5-3-4-8(6-9)10(12)7-11(13)15-2/h3-6,10,12H,7H2,1-2H3
InchiKey:	FNBHACUOQNHQRF-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COC(=O)CC(O)c1cccc(OC)c1
Mol. weight [g/mol]:	210.23

Physical Properties

Property code	Value	Unit	Source
gf	-333.66	kJ/mol	Joback Method
hf	-579.84	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	70.88	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.292		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1634.00		NIST Webbook
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tb	673.19	K	Joback Method
tc	872.12	K	Joback Method
tf	392.88	K	Joback Method
vc	0.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.11	J/molxK	673.19	Joback Method
cpg	476.04	J/molxK	838.96	Joback Method
cpg	467.00	J/molxK	805.81	Joback Method
cpg	457.29	J/molxK	772.65	Joback Method
cpg	446.91	J/molxK	739.50	Joback Method
cpg	435.85	J/molxK	706.34	Joback Method
cpg	484.42	J/molxK	872.12	Joback Method
dvisc	0.0000389	Paxs	673.19	Joback Method

dvisc	0.0000578	Paxs	626.47	Joback Method
dvisc	0.0000916	Paxs	579.75	Joback Method
dvisc	0.0001572	Paxs	533.04	Joback Method
dvisc	0.0002995	Paxs	486.32	Joback Method
dvisc	0.0006544	Paxs	439.60	Joback Method
dvisc	0.0017217	Paxs	392.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R106753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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