

m-Anisic acid, but-3-yn-2-yl ester

Inchi:	InChI=1S/C12H12O3/c1-4-9(2)15-12(13)10-6-5-7-11(8-10)14-3/h1,5-9H,2-3H3
InchiKey:	LZYKATSAEGECCP-UHFFFAOYSA-N
Formula:	C12H12O3
SMILES:	C#CC(C)OC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	204.22

Physical Properties

Property code	Value	Unit	Source
gf	34.65	kJ/mol	Joback Method
hf	-156.35	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	56.28	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	1.874		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	594.01	K	Joback Method
tc	817.42	K	Joback Method
tf	390.30	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.62	J/molxK	594.01	Joback Method
cpg	392.31	J/molxK	631.25	Joback Method
cpg	405.19	J/molxK	668.48	Joback Method
cpg	417.27	J/molxK	705.72	Joback Method
cpg	428.56	J/molxK	742.95	Joback Method
cpg	439.07	J/molxK	780.19	Joback Method
cpg	448.81	J/molxK	817.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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