

m-Anisic acid, oct-3-en-2-yl ester

Inchi:	InChI=1S/C16H22O3/c1-4-5-6-7-9-13(2)19-16(17)14-10-8-11-15(12-14)18-3/h7-13H,4-6H
InchiKey:	ILFVQCDCZZNIV-VQHVLOKHSA-N
Formula:	C16H22O3
SMILES:	CCCCC=CC(C)OC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	262.34

Physical Properties

Property code	Value	Unit	Source
gf	-74.52	kJ/mol	Joback Method
hf	-413.59	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.987		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1932.80		NIST Webbook
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tb	699.57	K	Joback Method
tc	904.52	K	Joback Method
tf	383.33	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.00	J/molxK	699.57	Joback Method
cpg	622.45	J/molxK	733.73	Joback Method
cpg	637.93	J/molxK	767.89	Joback Method
cpg	652.45	J/molxK	802.04	Joback Method
cpg	666.05	J/molxK	836.20	Joback Method
cpg	678.75	J/molxK	870.36	Joback Method
cpg	690.57	J/molxK	904.52	Joback Method
dvisc	0.0011364	Paxs	383.33	Joback Method

dvisc	0.0005496	Paxs	436.04	Joback Method
dvisc	0.0003109	Paxs	488.74	Joback Method
dvisc	0.0001965	Paxs	541.45	Joback Method
dvisc	0.0001347	Paxs	594.16	Joback Method
dvisc	0.0000982	Paxs	646.86	Joback Method
dvisc	0.0000751	Paxs	699.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292595&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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