

o-Anisic acid, 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C16H16O3/c1-11-8-12(2)10-13(9-11)19-16(17)14-6-4-5-7-15(14)18-3/h4-10H,1
InchiKey:	MXRXHWVGEIRHMR-UHFFFAOYSA-N
Formula:	C16H16O3
SMILES:	COc1ccccc1C(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	256.30

Physical Properties

Property code	Value	Unit	Source
gf	-59.15	kJ/mol	Joback Method
hf	-311.94	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.531		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2061.00		NIST Webbook
tb	732.49	K	Joback Method
tc	964.63	K	Joback Method
tf	454.87	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.39	J/molxK	732.49	Joback Method
cpg	557.61	J/molxK	771.18	Joback Method
cpg	571.68	J/molxK	809.87	Joback Method
cpg	584.61	J/molxK	848.56	Joback Method
cpg	596.44	J/molxK	887.25	Joback Method
cpg	607.15	J/molxK	925.94	Joback Method
cpg	616.78	J/molxK	964.63	Joback Method
dvisc	0.0006069	Paxs	454.87	Joback Method
dvisc	0.0003867	Paxs	501.14	Joback Method

dvisc	0.0002659	Paxs	547.41	Joback Method
dvisc	0.0001938	Paxs	593.68	Joback Method
dvisc	0.0001479	Paxs	639.95	Joback Method
dvisc	0.0001171	Paxs	686.22	Joback Method
dvisc	0.0000954	Paxs	732.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307791&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

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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