

o-Anisic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C15H14O3/c1-11-6-5-7-12(10-11)18-15(16)13-8-3-4-9-14(13)17-2/h3-10H,1-2H
InchiKey:	PZDHYNZJBITTKH-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	COc1ccccc1C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	242.27

Physical Properties

Property code	Value	Unit	Source
gf	-57.94	kJ/mol	Joback Method
hf	-279.83	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.223		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinsol	1964.00		NIST Webbook
tb	704.63	K	Joback Method
tc	940.44	K	Joback Method
tf	431.08	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.58	J/molxK	704.63	Joback Method
cpg	505.56	J/molxK	743.93	Joback Method
cpg	519.39	J/molxK	783.23	Joback Method
cpg	532.11	J/molxK	822.53	Joback Method
cpg	543.73	J/molxK	861.83	Joback Method
cpg	554.26	J/molxK	901.14	Joback Method
cpg	563.72	J/molxK	940.44	Joback Method
dvisc	0.0007551	Paxs	431.08	Joback Method
dvisc	0.0004658	Paxs	476.67	Joback Method

dvisc	0.0003126	Paxs	522.26	Joback Method
dvisc	0.0002237	Paxs	567.86	Joback Method
dvisc	0.0001682	Paxs	613.45	Joback Method
dvisc	0.0001316	Paxs	659.04	Joback Method
dvisc	0.0001063	Paxs	704.63	Joback Method

Sources

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=U307789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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