m-Anisic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H14O3/c1-11-5-3-8-14(9-11)18-15(16)12-6-4-7-13(10-12)17-2/h3-10H,1-2H
InchiKey: FEHHLAGRHWSQJW-UHFFFAOYSA-N
Formula: C15H14O3
SMILES: COc1cccc(C(=O)Oc2cccc(C)c2)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
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	704.63	K	Joback Method
tc	940.44	K	Joback Method
tf	431.08	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.58	J/mol×K	704.63	Joback Method
cpg	554.26	J/mol×K	901.14	Joback Method
cpg	543.73	J/mol×K	861.83	Joback Method
cpg	532.11	J/mol×K	822.53	Joback Method
cpg	519.39	J/mol×K	783.23	Joback Method
cpg	505.56	J/mol×K	743.93	Joback Method
cpg	563.72	J/mol×K	940.44	Joback Method
dvisc	0.0001063	Pa×s	704.63	Joback Method

dvisc	0.0001316	Pa×s	659.04	Joback Method
dvisc	0.0001682	Pa×s	613.45	Joback Method
dvisc	0.0002237	Pa×s	567.86	Joback Method
dvisc	0.0003126	Pa×s	522.26	Joback Method
dvisc	0.0004658	Pa×s	476.67	Joback Method
dvisc	0.0007551	Pa×s	431.08	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=U307798&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