m-Anisic acid, 2-adamantyl ester

Inchi: InChI=1S/C18H22O3/c1-20-16-4-2-3-13(10-16)18(19)21-17-14-6-11-5-12(8-14)9-15(17)7
InchiKey: RSTRVUVGKMYHEU-UHFFFAOYSA-N
Formula: C18H22O3
SMILES: COc1cccc(C(=O)OC2C3CC4CC(C3)CC2C4)c1
Mol. weight [g/mol]: 286.37

Physical Properties

Property code	Value	Unit	Source
gf	19.27	kJ/mol	Joback Method
hf	-395.25	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.677		Crippen Method
mcvol	221.450	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2395.80		NIST Webbook
tb	756.76	K	Joback Method
tc	987.36	K	Joback Method
tf	467.77	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.35	J/mol×K	756.76	Joback Method
cpg	723.04	J/mol×K	795.19	Joback Method
cpg	741.32	J/mol×K	833.63	Joback Method
cpg	758.30	J/mol×K	872.06	Joback Method
cpg	774.07	J/mol×K	910.49	Joback Method
cpg	788.75	J/mol×K	948.92	Joback Method
cpg	802.43	J/mol×K	987.36	Joback Method
dvisc	0.0032839	Pa×s	467.77	Joback Method
dvisc	0.0028853	Pa×s	515.93	Joback Method

dvisc	0.0025918	Pa×s	564.10	Joback Method
dvisc	0.0023677	Pa×s	612.27	Joback Method
dvisc	0.0021918	Pa×s	660.43	Joback Method
dvisc	0.0020503	Pa×s	708.60	Joback Method
dvisc	0.0019343	Pa×s	756.76	Joback Method

Sources

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=U292252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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