m-Anisic acid, cyclobutyl ester

Inchi: InChI=1S/C12H14O3/c1-14-11-7-2-4-9(8-11)12(13)15-10-5-3-6-10/h2,4,7-8,10H,3,5-6H2
InchiKey: FNCNTMFPAUQCCX-UHFFFAOYSA-N
Formula: C12H14O3
SMILES: COc1cccc(C(=O)OC2CCC2)c1
Mol. weight [g/mol]: 206.24

Physical Properties

Property code	Value	Unit	Source
gf	-137.33	kJ/mol	Joback Method
hf	-376.33	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	56.90	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.405		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1683.50		NIST Webbook
tb	615.34	K	Joback Method
tc	841.96	K	Joback Method
tf	372.75	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.05	J/mol×K	615.34	Joback Method
cpg	476.19	J/mol×K	804.19	Joback Method
cpg	464.13	J/mol×K	766.42	Joback Method
cpg	451.11	J/mol×K	728.65	Joback Method
cpg	437.11	J/mol×K	690.88	Joback Method
cpg	422.10	J/mol×K	653.11	Joback Method
cpg	487.32	J/mol×K	841.96	Joback Method
dvisc	0.0002682	Pa×s	615.34	Joback Method
dvisc	0.0003224	Pa×s	574.91	Joback Method

dvisc	0.0003985	Pa×s	534.48	Joback Method
dvisc	0.0005099	Pa×s	494.04	Joback Method
dvisc	0.0006818	Pa×s	453.61	Joback Method
dvisc	0.0009650	Pa×s	413.18	Joback Method
dvisc	0.0014728	Pa×s	372.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U292250&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