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
hf	-423.97	kJ/mol	Cheméo Relay (1.0)
hfus	20.50	kJ/mol	Joback Method
hvap	80.15	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
logp	2.405		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1683.50		NIST Webbook
tb	577.82	K	Cheméo Relay (1.0)
tc	793.64	K	Cheméo Relay (1.0)
tf	261.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.05	J/mol×K	615.34	Joback Method
cpg	487.32	J/mol×K	841.96	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
dvisc	0.0005099	Pa×s	494.04	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	0.0014728	Pa×s	372.75	Joback Method
dvisc	0.0006818	Pa×s	453.61	Joback Method
dvisc	0.0009650	Pa×s	413.18	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292250&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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