m-Toluic acid, cyclobutyl ester

Other names: m-toluylic acid, cyclobutyl ester
Inchi: InChI=1S/C12H14O2/c1-9-4-2-5-10(8-9)12(13)14-11-6-3-7-11/h2,4-5,8,11H,3,6-7H2,1H3
InchiKey: YEIVCBOAULAPEE-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: Cc1cccc(C(=O)OC2CCC2)c1
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-32.33	kJ/mol	Joback Method
hf	-244.11	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.704		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1532.10		NIST Webbook
rinpol	1532.10		NIST Webbook
tb	592.92	K	Joback Method
tc	822.69	K	Joback Method
tf	350.52	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.39	J/mol×K	592.92	Joback Method
cpg	452.21	J/mol×K	784.40	Joback Method
cpg	439.87	J/mol×K	746.10	Joback Method
cpg	426.56	J/mol×K	707.81	Joback Method
cpg	412.25	J/mol×K	669.51	Joback Method
cpg	396.87	J/mol×K	631.22	Joback Method
cpg	463.63	J/mol×K	822.69	Joback Method

dvisc	0.0003270	Pa×s	592.92	Joback Method
dvisc	0.0003929	Pa×s	552.52	Joback Method
dvisc	0.0004859	Pa×s	512.12	Joback Method
dvisc	0.0006232	Pa×s	471.72	Joback Method
dvisc	0.0008375	Pa×s	431.32	Joback Method
dvisc	0.0011964	Pa×s	390.92	Joback Method
dvisc	0.0018554	Pa×s	350.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292232&Units=SI
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

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