Cyclopropanecarboxylic acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C12H14O2/c1-8-4-3-5-11(9(8)2)14-12(13)10-6-7-10/h3-5,10H,6-7H2,1-2H3
InchiKey: IKNGHLJKRKVYEC-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: Cc1cccc(OC(=O)C2CC2)c1C
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-29.86	kJ/mol	Joback Method
hf	-249.42	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	54.97	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.619		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rinpol	1549.00		NIST Webbook
tb	593.63	K	Joback Method
tc	816.63	K	Joback Method
tf	366.56	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.84	J/mol×K	593.63	Joback Method
cpg	394.12	J/mol×K	630.80	Joback Method
cpg	408.45	J/mol×K	667.96	Joback Method
cpg	421.86	J/mol×K	705.13	Joback Method
cpg	434.40	J/mol×K	742.30	Joback Method
cpg	446.12	J/mol×K	779.46	Joback Method
cpg	457.06	J/mol×K	816.63	Joback Method
dvisc	0.0014969	Pa×s	366.56	Joback Method
dvisc	0.0010952	Pa×s	404.40	Joback Method

dvisc	0.0008454	Pa×s	442.25	Joback Method
dvisc	0.0006797	Pa×s	480.10	Joback Method
dvisc	0.0005642	Pa×s	517.94	Joback Method
dvisc	0.0004804	Pa×s	555.78	Joback Method
dvisc	0.0004175	Pa×s	593.63	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=U354662&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