Cyclobutanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H16O2/c1-9-6-10(2)8-12(7-9)15-13(14)11-4-3-5-11/h6-8,11H,3-5H2,1-2H3
InchiKey: SURSLDJUSQACFX-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: Cc1cc(C)cc(OC(=O)C2CCC2)c1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-33.54	kJ/mol	Joback Method
hf	-276.22	kJ/mol	Joback Method
hfus	21.51	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.009		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1579.00		NIST Webbook
tb	620.78	K	Joback Method
tc	847.11	K	Joback Method
tf	374.31	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	620.78	Joback Method
cpg	446.49	J/mol×K	658.50	Joback Method
cpg	462.20	J/mol×K	696.22	Joback Method
cpg	476.88	J/mol×K	733.94	Joback Method
cpg	490.56	J/mol×K	771.67	Joback Method
cpg	503.29	J/mol×K	809.39	Joback Method
cpg	515.11	J/mol×K	847.11	Joback Method
dvisc	0.0015357	Pa×s	374.31	Joback Method
dvisc	0.0010248	Pa×s	415.39	Joback Method

dvisc	0.0007354	Pa×s	456.47	Joback Method
dvisc	0.0005575	Pa×s	497.54	Joback Method
dvisc	0.0004409	Pa×s	538.62	Joback Method
dvisc	0.0003605	Pa×s	579.70	Joback Method
dvisc	0.0003026	Pa×s	620.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307438&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