

Cyclopropanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C12H14O2/c1-8-5-9(2)7-11(6-8)14-12(13)10-3-4-10/h5-7,10H,3-4H2,1-2H3
InchiKey:	TYGXPZHSCQEDFV-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	<chem>Cc1cc(C)cc(OC(=O)C2CC2)c1</chem>
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
rinqol	1487.00		NIST Webbook
tb	593.63	K	Joback Method
tc	816.63	K	Joback Method
tf	366.56	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0008454	Paxs	442.25	Joback Method
dvisc	0.0006797	Paxs	480.10	Joback Method
dvisc	0.0005642	Paxs	517.94	Joback Method
dvisc	0.0004804	Paxs	555.78	Joback Method
dvisc	0.0004175	Paxs	593.63	Joback Method

Sources

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=U307523&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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