

o-Toluic acid, cyclobutyl ester

Other names:	o-toluylic acid, cyclobutyl ester
Inchi:	InChI=1S/C12H14O2/c1-9-5-2-3-8-11(9)12(13)14-10-6-4-7-10/h2-3,5,8,10H,4,6-7H2,1H3
InchiKey:	DBFKZOIUYMDLIP-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	<chem>Cc1ccccc1C(=O)OC1CCC1</chem>
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	1501.20		NIST Webbook
tb	592.92	K	Joback Method
tc	822.69	K	Joback Method
tf	350.52	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.39	J/molxK	592.92	Joback Method
cpg	396.87	J/molxK	631.22	Joback Method
cpg	412.25	J/molxK	669.51	Joback Method
cpg	426.56	J/molxK	707.81	Joback Method
cpg	439.87	J/molxK	746.10	Joback Method
cpg	452.21	J/molxK	784.40	Joback Method
cpg	463.63	J/molxK	822.69	Joback Method
dvisc	0.0018554	Paxs	350.52	Joback Method

dvisc	0.0011964	Paxs	390.92	Joback Method
dvisc	0.0008375	Paxs	431.32	Joback Method
dvisc	0.0006232	Paxs	471.72	Joback Method
dvisc	0.0004859	Paxs	512.12	Joback Method
dvisc	0.0003929	Paxs	552.52	Joback Method
dvisc	0.0003270	Paxs	592.92	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=U292223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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