Cyclobutanecarboxylic acid, phenyl ester

Inchi: InChI=1S/C11H12O2/c12-11(9-5-4-6-9)13-10-7-2-1-3-8-10/h1-3,7-9H,4-6H2
InchiKey: QSPUUVAPVKVXFB-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: O=C(Oc1ccccc1)C1CCC1
Mol. weight [g/mol]: 176.21
CAS: 30466-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-31.12	kJ/mol	Joback Method
hf	-212.00	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	51.60	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.392		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
tb	565.06	K	Joback Method
tc	798.36	K	Joback Method
tf	326.73	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.53	J/mol×K	565.06	Joback Method
cpg	402.32	J/mol×K	759.48	Joback Method
cpg	390.43	J/mol×K	720.59	Joback Method
cpg	377.56	J/mol×K	681.71	Joback Method
cpg	363.65	J/mol×K	642.83	Joback Method
cpg	348.66	J/mol×K	603.94	Joback Method
cpg	413.29	J/mol×K	798.36	Joback Method

dvisc	0.0003529	Pa×s	565.06	Joback Method
dvisc	0.0004282	Pa×s	525.34	Joback Method
dvisc	0.0005363	Pa×s	485.62	Joback Method
dvisc	0.0006991	Pa×s	445.89	Joback Method
dvisc	0.0009599	Pa×s	406.17	Joback Method
dvisc	0.0014118	Pa×s	366.45	Joback Method
dvisc	0.0022805	Pa×s	326.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30466310&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