Cyclopentanecarboxylic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C12H12Cl2O2/c13-10-6-5-9(7-11(10)14)16-12(15)8-3-1-2-4-8/h5-8H,1-4H2
InchiKey: CIKRVIKIBNQLQZ-UHFFFAOYSA-N
Formula: C12H12Cl2O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C1CCCC1
Mol. weight [g/mol]: 259.13

Physical Properties

Property code	Value	Unit	Source
gf	-77.92	kJ/mol	Joback Method
hf	-293.22	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.089		Crippen Method
mcvol	177.240	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1849.00		NIST Webbook
tb	677.03	K	Joback Method
tc	921.84	K	Joback Method
tf	419.36	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.39	J/mol×K	677.03	Joback Method
cpg	449.07	J/mol×K	717.83	Joback Method
cpg	462.59	J/mol×K	758.63	Joback Method
cpg	475.00	J/mol×K	799.43	Joback Method
cpg	486.34	J/mol×K	840.23	Joback Method
cpg	496.64	J/mol×K	881.03	Joback Method
cpg	505.95	J/mol×K	921.84	Joback Method
dvisc	0.0014060	Pa×s	419.36	Joback Method
dvisc	0.0009042	Pa×s	462.31	Joback Method

dvisc	0.0006268	Pa×s	505.25	Joback Method
dvisc	0.0004602	Pa×s	548.19	Joback Method
dvisc	0.0003533	Pa×s	591.14	Joback Method
dvisc	0.0002812	Pa×s	634.09	Joback Method
dvisc	0.0002304	Pa×s	677.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307579&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

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