3-Cyclopentylpropionic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H16Cl2O2/c15-12-7-6-11(9-13(12)16)18-14(17)8-5-10-3-1-2-4-10/h6-7,9-1

InchiKey: JPOVKVUFJRAFMA-UHFFFAOYSA-N

Formula: C14H16Cl2O2

SMILES: O=C(CCC1CCCC1)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 287.18

Physical Properties

Property code	Value	Unit	Source
gf	-61.08	kJ/mol	Joback Method
hf	-334.50	kJ/mol	Joback Method
hfus	30.39	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.869		Crippen Method
mcvol	205.420	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	722.79	K	Joback Method
tc	957.71	K	Joback Method
tf	441.90	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.43	J/mol×K	722.79	Joback Method
cpg	553.95	J/mol×K	761.94	Joback Method
cpg	568.29	J/mol×K	801.10	Joback Method
cpg	581.47	J/mol×K	840.25	Joback Method
cpg	593.56	J/mol×K	879.40	Joback Method
cpg	604.59	J/mol×K	918.56	Joback Method
cpg	614.61	J/mol×K	957.71	Joback Method
dvisc	0.0012577	Pa×s	441.90	Joback Method

dvisc	0.0007838	Pa×s	488.71	Joback Method
dvisc	0.0005306	Pa×s	535.53	Joback Method
dvisc	0.0003824	Pa×s	582.35	Joback Method
dvisc	0.0002894	Pa×s	629.16	Joback Method
dvisc	0.0002276	Pa×s	675.97	Joback Method
dvisc	0.0001847	Pa×s	722.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307135&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