3-Cyclopentylpropionic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H15Cl3O2/c15-10-7-12(17)13(8-11(10)16)19-14(18)6-5-9-3-1-2-4-9/h7-9H,
InchiKey: XIBYBGGUAYSUMU-UHFFFAOYSA-N
Formula: C14H15Cl3O2
SMILES: O=C(CCC1CCCC1)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 321.63

Physical Properties

Property code	Value	Unit	Source
gf	-82.64	kJ/mol	Joback Method
hf	-361.71	kJ/mol	Joback Method
hfus	34.20	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.523		Crippen Method
mcvol	217.660	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	765.20	K	Joback Method
tc	1003.27	K	Joback Method
tf	484.34	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.24	J/mol×K	765.20	Joback Method
cpg	576.31	J/mol×K	804.88	Joback Method
cpg	589.23	J/mol×K	844.56	Joback Method
cpg	601.04	J/mol×K	884.24	Joback Method
cpg	611.79	J/mol×K	923.92	Joback Method
cpg	621.52	J/mol×K	963.59	Joback Method
cpg	630.27	J/mol×K	1003.27	Joback Method
dvisc	0.0009588	Pa×s	484.34	Joback Method

dvisc	0.0006307	Pa×s	531.15	Joback Method
dvisc	0.0004441	Pa×s	577.96	Joback Method
dvisc	0.0003295	Pa×s	624.77	Joback Method
dvisc	0.0002549	Pa×s	671.58	Joback Method
dvisc	0.0002039	Pa×s	718.39	Joback Method
dvisc	0.0001676	Pa×s	765.20	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354059&Units=SI

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