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

Inchi: InChI=1S/C15H11Cl3O2/c16-11-8-13(18)14(9-12(11)17)20-15(19)7-6-10-4-2-1-3-5-10/h1

InchiKey: NBCATOXCSOXZTK-UHFFFAOYSA-N

Formula: C15H11Cl3O2

SMILES: O=C(CCc1ccccc1)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 329.61

Physical Properties

Property code	Value	Unit	Source
gf	1.64	kJ/mol	Joback Method
hf	-206.30	kJ/mol	Joback Method
hfus	36.90	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.185		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	799.48	K	Joback Method
tc	1046.25	K	Joback Method
tf	511.13	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.35	J/mol×K	799.48	Joback Method
cpg	580.23	J/mol×K	1005.12	Joback Method
cpg	572.81	J/mol×K	964.00	Joback Method
cpg	564.46	J/mol×K	922.87	Joback Method
cpg	555.13	J/mol×K	881.74	Joback Method
cpg	544.78	J/mol×K	840.61	Joback Method
cpg	586.75	J/mol×K	1046.25	Joback Method
dvisc	0.0001026	Pa×s	799.48	Joback Method

dvisc	0.0001255	Pa×s	751.42	Joback Method
dvisc	0.0001578	Pa×s	703.36	Joback Method
dvisc	0.0002052	Pa×s	655.31	Joback Method
dvisc	0.0002782	Pa×s	607.25	Joback Method
dvisc	0.0003973	Pa×s	559.19	Joback Method
dvisc	0.0006067	Pa×s	511.13	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=U354745&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