3-Phenylpropionic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C15H10Cl4O2/c16-10-8-11(17)15(14(19)13(10)18)21-12(20)7-6-9-4-2-1-3-5-9/

InchiKey: VQWOGTZZJINORW-UHFFFAOYSA-N

Formula: C15H10Cl4O2

SMILES: O=C(CCc1ccccc1)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 364.05

Physical Properties

Property code	Value	Unit	Source
gf	-19.92	kJ/mol	Joback Method
hf	-233.51	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.838		Crippen Method
mcvol	231.090	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2569.00		NIST Webbook
tb	841.89	K	Joback Method
tc	1091.27	K	Joback Method
tf	553.57	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.51	J/mol×K	841.89	Joback Method
cpg	592.13	J/mol×K	1049.70	Joback Method
cpg	585.91	J/mol×K	1008.14	Joback Method
cpg	578.77	J/mol×K	966.58	Joback Method
cpg	570.68	J/mol×K	925.02	Joback Method
cpg	561.61	J/mol×K	883.45	Joback Method
cpg	597.49	J/mol×K	1091.27	Joback Method
dvisc	0.0000913	Pa×s	841.89	Joback Method
dvisc	0.0001104	Pa×s	793.84	Joback Method

dvisc	0.0001368	Pa×s	745.78	Joback Method
dvisc	0.0001745	Pa×s	697.73	Joback Method
dvisc	0.0002308	Pa×s	649.68	Joback Method
dvisc	0.0003192	Pa×s	601.62	Joback Method
dvisc	0.0004671	Pa×s	553.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354746&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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