4-Methylbenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H9Cl3O2/c1-8-2-4-9(5-3-8)14(18)19-13-7-11(16)10(15)6-12(13)17/h2-7H,1

InchiKey: XHTJGHOZWZWGLE-UHFFFAOYSA-N

Formula: C14H9Cl3O2

SMILES: Cc1ccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)cc1

Mol. weight [g/mol]: 315.58

Physical Properties

Property code	Value	Unit	Source
gf	-16.41	kJ/mol	Joback Method
hf	-197.13	kJ/mol	Joback Method
hfus	33.92	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.174		Crippen Method
mcvol	204.760	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook
tb	781.58	K	Joback Method
tc	1034.18	K	Joback Method
tf	512.38	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.12	J/mol×K	781.58	Joback Method
cpg	490.00	J/mol×K	823.68	Joback Method
cpg	499.85	J/mol×K	865.78	Joback Method
cpg	508.69	J/mol×K	907.88	Joback Method
cpg	516.57	J/mol×K	949.98	Joback Method
cpg	523.52	J/mol×K	992.08	Joback Method
cpg	529.55	J/mol×K	1034.18	Joback Method
dvisc	0.0005792	Pa×s	512.38	Joback Method

dvisc	0.0003990	Pa×s	557.25	Joback Method
dvisc	0.0002905	Pa×s	602.11	Joback Method
dvisc	0.0002210	Pa×s	646.98	Joback Method
dvisc	0.0001742	Pa×s	691.85	Joback Method
dvisc	0.0001414	Pa×s	736.71	Joback Method
dvisc	0.0001175	Pa×s	781.58	Joback Method

Sources

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=U354157&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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