

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

Inchi:	InChI=1S/C14H9Cl3O3/c1-19-9-4-2-8(3-5-9)14(18)20-13-7-11(16)10(15)6-12(13)17/h2-7
InchiKey:	IGWHCSI AKZETGT-UHFFFAOYSA-N
Formula:	C14H9Cl3O3
SMILES:	COc1ccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	331.58

Physical Properties

Property code	Value	Unit	Source
gf	-121.41	kJ/mol	Joback Method
hf	-329.35	kJ/mol	Joback Method
hfus	35.11	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.875		Crippen Method
mvol	210.630	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	2508.00		NIST Webbook
tb	804.00	K	Joback Method
tc	1052.68	K	Joback Method
tf	534.61	K	Joback Method
vc	0.792	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.00	J/molxK	804.00	Joback Method
cpg	513.51	J/molxK	845.45	Joback Method
cpg	522.93	J/molxK	886.89	Joback Method
cpg	531.29	J/molxK	928.34	Joback Method
cpg	538.58	J/molxK	969.78	Joback Method
cpg	544.80	J/molxK	1011.23	Joback Method
cpg	549.98	J/molxK	1052.68	Joback Method
dvisc	0.0004288	Paxs	534.61	Joback Method
dvisc	0.0002987	Paxs	579.51	Joback Method

dvisc	0.0002192	Paxs	624.41	Joback Method
dvisc	0.0001676	Paxs	669.31	Joback Method
dvisc	0.0001326	Paxs	714.20	Joback Method
dvisc	0.0001079	Paxs	759.10	Joback Method
dvisc	0.0000898	Paxs	804.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U360532&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

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