

Benzoic acid, 3-methyl-, 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C14H8Cl4O2/c1-7-3-2-4-8(5-7)14(19)20-13-10(16)6-9(15)11(17)12(13)18/h2-6
InchiKey:	QZOPQAMVANOJJE-UHFFFAOYSA-N
Formula:	C14H8Cl4O2
SMILES:	Cc1cccc(C(=O)Oc2c(Cl)cc(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]:	350.02

Physical Properties

Property code	Value	Unit	Source
gf	-37.97	kJ/mol	Joback Method
hf	-224.34	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.828		Crippen Method
mvol	217.000	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2454.00		NIST Webbook
tb	823.99	K	Joback Method
tc	1078.98	K	Joback Method
tf	554.82	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.61	J/mol×K	823.99	Joback Method
cpg	506.20	J/mol×K	866.49	Joback Method
cpg	514.79	J/mol×K	908.99	Joback Method
cpg	522.41	J/mol×K	951.48	Joback Method
cpg	529.08	J/mol×K	993.98	Joback Method
cpg	534.83	J/mol×K	1036.48	Joback Method
cpg	539.67	J/mol×K	1078.98	Joback Method
dvisc	0.0004583	Paxs	554.82	Joback Method
dvisc	0.0003275	Paxs	599.68	Joback Method

dvisc	0.0002452	Paxs	644.54	Joback Method
dvisc	0.0001906	Paxs	689.40	Joback Method
dvisc	0.0001528	Paxs	734.27	Joback Method
dvisc	0.0001257	Paxs	779.13	Joback Method
dvisc	0.0001056	Paxs	823.99	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=U355715&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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