Tetrabromophenolphthalein, ethyl ester

Other names:	ethyl 2-[(3,5-dibromo-4-hydroxyphenyl)(3,5-dibromo-4-oxo-2,5-cyclohexadien-1-ylidene)methyl
Inchi:	InChI=1S/C22H14Br4O4/c1-2-30-22(29)14-6-4-3-5-13(14)19(11-7-15(23)20(27)16(24)8-
InchiKey:	SQFXATUXPUCFFO-UHFFFAOYSA-N
Formula:	C22H14Br4O4
SMILES:	CCOC(=O)c1ccccc1C(=C1C=C(Br)C(=O)C(Br)=C1)c1cc(Br)c(O)c(Br)c1
Mol. weight [g/mol]:	661.96
CAS:	1176-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-13.83	kJ/mol	Joback Method
hf	-279.73	kJ/mol	Joback Method
hfus	60.31	kJ/mol	Joback Method
hvap	126.77	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	7.036		Crippen Method
mcvol	334.440	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	1299.45	K	Joback Method
tc	1604.46	K	Joback Method
tf	953.98	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.25	J/mol×K	1299.45	Joback Method
cpg	944.28	J/mol×K	1350.28	Joback Method
cpg	959.03	J/mol×K	1401.12	Joback Method
cpg	974.75	J/mol×K	1451.95	Joback Method
cpg	991.71	J/mol×K	1502.79	Joback Method
cpg	1010.15	J/mol×K	1553.62	Joback Method
cpg	1030.31	J/mol×K	1604.46	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=C1176745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume