1-Naphthoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C17H8Cl4O2/c18-12-8-13(19)16(15(21)14(12)20)23-17(22)11-7-3-5-9-4-1-2-6-

InchiKey: OHNLBGHBSDGQKI-UHFFFAOYSA-N

Formula: C17H8Cl4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1cccc2ccccc12

Mol. weight [g/mol]: 386.06

Physical Properties

Property code	Value	Unit	Source
gf	93.94	kJ/mol	Joback Method
hf	-95.19	kJ/mol	Joback Method
hfus	42.52	kJ/mol	Joback Method
hvap	89.63	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.673		Crippen Method
mcvol	239.810	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	3002.00		NIST Webbook
tb	911.61	K	Joback Method
tc	1177.04	K	Joback Method
tf	621.33	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.78	J/mol×K	911.61	Joback Method
cpg	585.81	J/mol×K	955.85	Joback Method
cpg	593.96	J/mol×K	1000.09	Joback Method
cpg	601.30	J/mol×K	1044.32	Joback Method
cpg	607.93	J/mol×K	1088.56	Joback Method
cpg	613.94	J/mol×K	1132.80	Joback Method
cpg	619.42	J/mol×K	1177.04	Joback Method
dvisc	0.0005156	Pa×s	621.33	Joback Method
dvisc	0.0003865	Pa×s	669.71	Joback Method

dvisc	0.0003012	Pa×s	718.09	Joback Method
dvisc	0.0002423	Pa×s	766.47	Joback Method
dvisc	0.0002000	Pa×s	814.85	Joback Method
dvisc	0.0001686	Pa×s	863.23	Joback Method
dvisc	0.0001448	Pa×s	911.61	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=U355696&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