1-Naphthoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C17H9Cl3O2/c18-13-8-15(20)16(9-14(13)19)22-17(21)12-7-3-5-10-4-1-2-6-11(
InchiKey: ARGSNZNGENVAPU-UHFFFAOYSA-N
Formula: C17H9Cl3O2
SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1cccc2ccccc12
Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	115.50	kJ/mol	Joback Method
hf	-67.98	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	84.59	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.019		Crippen Method
mcvol	227.570	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook
tb	869.20	K	Joback Method
tc	1132.67	K	Joback Method
tf	578.89	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.03	J/mol×K	869.20	Joback Method
cpg	571.25	J/mol×K	913.11	Joback Method
cpg	580.50	J/mol×K	957.02	Joback Method
cpg	588.88	J/mol×K	1000.94	Joback Method
cpg	596.47	J/mol×K	1044.85	Joback Method
cpg	603.38	J/mol×K	1088.76	Joback Method
cpg	609.70	J/mol×K	1132.67	Joback Method
dvisc	0.0006244	Pa×s	578.89	Joback Method

dvisc	0.0004560	Pa×s	627.28	Joback Method
dvisc	0.0003484	Pa×s	675.66	Joback Method
dvisc	0.0002760	Pa×s	724.05	Joback Method
dvisc	0.0002250	Pa×s	772.43	Joback Method
dvisc	0.0001880	Pa×s	820.82	Joback Method
dvisc	0.0001602	Pa×s	869.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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