1-Naphthoic acid, 3,4-dichlorophenyl ester

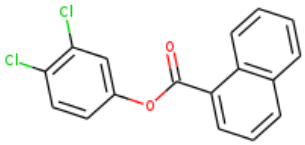
InChI: InChI=1S/C17H10Cl2O2/c18-15-9-8-12(10-16(15)19)21-17(20)14-7-3-5-11-4-1-2-6-13(11)14/h1-10H

InChI Key: OMRXSGMGDYFBMY-UHFFFAOYSA-N

Formula: C17H10Cl2O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc2ccccc21

Molecular Weight: 317.17



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	137.06	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-40.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.90	kJ/mol	Joback Method
$\Delta_{vap} H°$	79.54	kJ/mol	Joback Method
$logP_{oct/wat}$	5.37		Crippen Method
P_c	2460.47	kPa	Joback Method
T_{boil}	826.79	K	Joback Method
T_c	1088.26	K	Joback Method
T_{fus}	536.45	K	Joback Method
V_c	0.82	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	543.63	J/mol×K	826.79	Joback Method
η	0.00	Pa×s	826.79	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H10Cl2O2/c18-15-9-8-12(10-16(15)19)21-17(20)14-7-3-5-11-4-1-2-6-13(11)14/h1-10H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).