1-Naphthaleneacetic acid, 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H12Cl2O2/c19-15-9-4-10-16(18(15)20)22-17(21)11-13-7-3-6-12-5-1-2-8-14

InchiKey: GAISTWFBFLMFJV-UHFFFAOYSA-N

Formula: C18H12Cl2O2

SMILES: O=C(Cc1cccc2ccccc12)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	145.48	kJ/mol	Joback Method
hf	-61.41	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.295		Crippen Method
mcvol	229.420	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
tb	849.67	K	Joback Method
tc	1105.76	K	Joback Method
tf	547.72	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.65	J/mol×K	849.67	Joback Method
cpg	647.55	J/mol×K	1063.08	Joback Method
cpg	639.28	J/mol×K	1020.39	Joback Method
cpg	630.26	J/mol×K	977.71	Joback Method
cpg	620.38	J/mol×K	935.03	Joback Method
cpg	609.54	J/mol×K	892.35	Joback Method
cpg	655.16	J/mol×K	1105.76	Joback Method
dvisc	0.0001559	Pa×s	849.67	Joback Method

dvisc	0.0001854	Pa×s	799.35	Joback Method
dvisc	0.0002255	Pa×s	749.02	Joback Method
dvisc	0.0002822	Pa×s	698.70	Joback Method
dvisc	0.0003656	Pa×s	648.37	Joback Method
dvisc	0.0004948	Pa×s	598.05	Joback Method
dvisc	0.0007080	Pa×s	547.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415053&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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