

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(1
InchiKey:	OMRXSGMGDYFBMY-UHFFFAOYSA-N
Formula:	C17H10Cl2O2
SMILES:	O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc2ccccc12
Mol. weight [g/mol]:	317.17

Physical Properties

Property code	Value	Unit	Source
gf	137.06	kJ/mol	Joback Method
hf	-40.77	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.366		Crippen Method
mcvol	215.330	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinsol	2616.00		NIST Webbook
tb	826.79	K	Joback Method
tc	1088.26	K	Joback Method
tf	536.45	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.63	J/molxK	826.79	Joback Method
cpg	555.14	J/molxK	870.37	Joback Method
cpg	565.59	J/molxK	913.95	Joback Method
cpg	575.07	J/molxK	957.53	Joback Method
cpg	583.69	J/molxK	1001.11	Joback Method
cpg	591.54	J/molxK	1044.68	Joback Method
cpg	598.72	J/molxK	1088.26	Joback Method
dvisc	0.0007590	Paxs	536.45	Joback Method
dvisc	0.0005375	Paxs	584.84	Joback Method

dvisc	0.0004012	Paxs	633.23	Joback Method
dvisc	0.0003122	Paxs	681.62	Joback Method
dvisc	0.0002512	Paxs	730.01	Joback Method
dvisc	0.0002076	Paxs	778.40	Joback Method
dvisc	0.0001754	Paxs	826.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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