

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
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tb	869.20	K	Joback Method
tc	1132.67	K	Joback Method
tf	578.89	K	Joback Method
vc	0.865	m ³ /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	Paxs	578.89	Joback Method

dvisc	0.0004560	Paxs	627.28	Joback Method
dvisc	0.0003484	Paxs	675.66	Joback Method
dvisc	0.0002760	Paxs	724.05	Joback Method
dvisc	0.0002250	Paxs	772.43	Joback Method
dvisc	0.0001880	Paxs	820.82	Joback Method
dvisc	0.0001602	Paxs	869.20	Joback Method

Sources

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=U355695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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