1-Naphthoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C17H11ClO2/c18-13-8-10-14(11-9-13)20-17(19)16-7-3-5-12-4-1-2-6-15(12)16/
InchiKey: ZTNAIEDTVGAUOA-UHFFFAOYSA-N
Formula: C17H11ClO2
SMILES: O=C(Oc1ccc(Cl)cc1)c1cccc2ccccc12
Mol. weight [g/mol]: 282.72

Physical Properties

Property code	Value	Unit	Source
gf	158.62	kJ/mol	Joback Method
hf	-13.56	kJ/mol	Joback Method
hfus	31.09	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.712		Crippen Method
mcvol	203.090	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	784.38	K	Joback Method
tc	1043.72	K	Joback Method
tf	494.01	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.43	J/mol×K	784.38	Joback Method
cpg	578.35	J/mol×K	1000.49	Joback Method
cpg	569.49	J/mol×K	957.27	Joback Method
cpg	559.77	J/mol×K	914.05	Joback Method
cpg	549.09	J/mol×K	870.83	Joback Method
cpg	537.35	J/mol×K	827.60	Joback Method
cpg	586.46	J/mol×K	1043.72	Joback Method
dvisc	0.0001897	Pa×s	784.38	Joback Method

dvisc	0.0002266	Pa×s	735.99	Joback Method
dvisc	0.0002774	Pa×s	687.59	Joback Method
dvisc	0.0003503	Pa×s	639.20	Joback Method
dvisc	0.0004595	Pa×s	590.80	Joback Method
dvisc	0.0006327	Pa×s	542.41	Joback Method
dvisc	0.0009274	Pa×s	494.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307824&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