1-Naphthoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C19H16O2/c1-13-10-14(2)12-16(11-13)21-19(20)18-9-5-7-15-6-3-4-8-17(15)18
InchiKey: YSHJDUIJHHEDGD-UHFFFAOYSA-N
Formula: C19H16O2
SMILES: Cc1cc(C)cc(OC(=O)c2cccc3ccccc23)c1
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	177.76	kJ/mol	Joback Method
hf	-50.57	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.676		Crippen Method
mcvol	219.030	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2419.00		NIST Webbook
tb	797.69	K	Joback Method
tc	1045.30	K	Joback Method
tf	499.15	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.12	J/mol×K	797.69	Joback Method
cpg	671.11	J/mol×K	1004.03	Joback Method
cpg	660.57	J/mol×K	962.76	Joback Method
cpg	649.08	J/mol×K	921.49	Joback Method
cpg	636.57	J/mol×K	880.23	Joback Method
cpg	622.95	J/mol×K	838.96	Joback Method
cpg	680.80	J/mol×K	1045.30	Joback Method
dvisc	0.0001681	Pa×s	797.69	Joback Method
dvisc	0.0002000	Pa×s	747.93	Joback Method

dvisc	0.0002440	Pa×s	698.18	Joback Method
dvisc	0.0003067	Pa×s	648.42	Joback Method
dvisc	0.0004006	Pa×s	598.66	Joback Method
dvisc	0.0005492	Pa×s	548.91	Joback Method
dvisc	0.0008017	Pa×s	499.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307825&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