1-Naphthoic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C19H16O2/c1-2-14-7-5-10-16(13-14)21-19(20)18-12-6-9-15-8-3-4-11-17(15)18
InchiKey: VGMQRDQOHOKUKQ-UHFFFAOYSA-N
Formula: C19H16O2
SMILES: CCc1cccc(OC(=O)c2cccc3ccccc23)c1
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	187.39	kJ/mol	Joback Method
hf	-39.10	kJ/mol	Joback Method
hfus	32.08	kJ/mol	Joback Method
hvap	74.56	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.621		Crippen Method
mcvol	219.030	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	2528.00		NIST Webbook
tb	792.71	K	Joback Method
tc	1039.60	K	Joback Method
tf	486.63	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.37	J/mol×K	792.71	Joback Method
cpg	672.78	J/mol×K	998.45	Joback Method
cpg	662.15	J/mol×K	957.30	Joback Method
cpg	650.60	J/mol×K	916.15	Joback Method
cpg	638.01	J/mol×K	875.01	Joback Method
cpg	624.30	J/mol×K	833.86	Joback Method
cpg	682.57	J/mol×K	1039.60	Joback Method
dvisc	0.0001660	Pa×s	792.71	Joback Method
dvisc	0.0001997	Pa×s	741.70	Joback Method

dvisc	0.0002470	Pa×s	690.68	Joback Method
dvisc	0.0003161	Pa×s	639.67	Joback Method
dvisc	0.0004221	Pa×s	588.66	Joback Method
dvisc	0.0005954	Pa×s	537.64	Joback Method
dvisc	0.0009028	Pa×s	486.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355692&Units=SI

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