1-Naphthoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C17H11NO4/c19-17(22-14-10-8-13(9-11-14)18(20)21)16-7-3-5-12-4-1-2-6-15(
InchiKey: LFZNDEUETPVUAT-UHFFFAOYSA-N
Formula: C17H11NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc2ccccc12
Mol. weight [g/mol]: 293.27

Physical Properties

Property code	Value	Unit	Source
gf	206.10	kJ/mol	Joback Method
hf	-8.58	kJ/mol	Joback Method
hfus	38.26	kJ/mol	Joback Method
hvap	86.70	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	3.967		Crippen Method
mcvol	208.270	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	898.79	K	Joback Method
tc	1171.23	K	Joback Method
tf	607.70	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.90	J/mol×K	898.79	Joback Method
cpg	604.02	J/mol×K	944.20	Joback Method
cpg	614.05	J/mol×K	989.60	Joback Method
cpg	623.12	J/mol×K	1035.01	Joback Method
cpg	631.35	J/mol×K	1080.42	Joback Method
cpg	638.88	J/mol×K	1125.82	Joback Method
cpg	645.83	J/mol×K	1171.23	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=U307829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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