3-Nitro-1,8-Naphthalic anhydride

Other names: Naphthalic anhydride, 3-nitro-
1H,3H-Naphtho(1,8-cd)pyran-1,3-dione, 5-nitro-
3-Nitronaphthalic anhydride
Inchi: InChI=1S/C12H5NO5/c14-11-8-3-1-2-6-4-7(13(16)17)5-9(10(6)8)12(15)18-11/h1-5H
InchiKey: FLFLZYYDLIKGJQ-UHFFFAOYSA-N
Formula: C12H5NO5
SMILES: O=C1OC(=O)c2cc([N+](=O)[O-])cc3cccc1c23
Mol. weight [g/mol]: 243.17

Physical Properties

Property code	Value	Unit	Source
hfus	32.15	kJ/mol	Joback Method
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	2.059		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
tb	661.47	K	Cheméo Relay (1.0)
tf	461.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.32	J/mol×K	860.40	Joback Method
cpg	441.22	J/mol×K	908.36	Joback Method
cpg	450.00	J/mol×K	956.33	Joback Method
cpg	457.73	J/mol×K	1004.29	Joback Method
cpg	464.45	J/mol×K	1052.25	Joback Method
cpg	470.22	J/mol×K	1100.21	Joback Method
cpg	475.08	J/mol×K	1148.18	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3027381&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point