1,4,5,8-Naphthalenetetracarboxylic dianhydride

Other names: Naphthalene-1,4,5,8-tetracarboxylic dianhydride
[2]Benzopyrano[6,5,4-def][2]benzopyran-1,3,6,8-tetrone
Naphthalenetetracarboxylic dianhydride
1,4,5,8-Naphthalenetetracarboxylic acid anhydride
1,4,5,8-Naphthalenetetracarboxylic acid dianhydride
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-dianhydride
1,8:4,5-Naphthalenetetracarboxylic dianhydride
2,7-Dioxapyrene-1,3,6,8-tetrone
1,4,5,8-Naphthalenetetracarboxylic acid, 1,8:4,5-dianhydride
NSC 84241
NTCDA
naphthalene-1,8:4,5-tetracarboxylic dianhydride

Inchi: InChI=1S/C14H4O6/c15-11-5-1-2-6-10-8(14(18)20-12(6)16)4-3-7(9(5)10)13(17)19-11/h1

InchiKey: YTVNOVQHSGMMOV-UHFFFAOYSA-N

Formula: C14H4O6

SMILES: O=C1OC(=O)c2ccc3c4c(ccc1c24)C(=O)OC3=O

Mol. weight [g/mol]: 268.18

CAS: 81-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-278.14	kJ/mol	Joback Method
hf	-579.09	kJ/mol	Joback Method
hfus	29.65	kJ/mol	Joback Method
hvap	79.77	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	1.461		Crippen Method
mcvol	161.200	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	933.30	K	Joback Method
tc	1222.26	K	Joback Method
tf	727.12	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.48	J/mol×K	933.30	Joback Method
cpg	498.71	J/mol×K	981.46	Joback Method
cpg	506.37	J/mol×K	1029.62	Joback Method
cpg	512.43	J/mol×K	1077.78	Joback Method
cpg	516.85	J/mol×K	1125.94	Joback Method
cpg	519.60	J/mol×K	1174.10	Joback Method
cpg	520.64	J/mol×K	1222.26	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=C81301&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume