3,4,9,10-Perylenetetracarboxylic dianhydride

Other names:	Perylene-3,4,9,10-tetracarboxylic dianhydride
	3,4,9,10-Perylenetetracarboxylic 3,4:9,10-dianhydride
	Perylo[3,4-cd:9,10-c'd']dipyran-1,3,8,10-tetrone
	Perylene-3,4,9,10-tetracarboxylic 3,4:9,10-dianhydride
	Perylenetetracarboxylic acid dianhydride
	Perylenetetracarboxylic anhydride
	3,4:9,10-Perylenetetracarboxylic anhydride
	1,3,8,10-Tetraoxaperylo[3,4-cd:9,10-c'd']dipyran
	NSC 79895
	Pigment Red 224
	Irgazin Red BPT
	C.I. Pigment Red 224
	perylene-3,4:9,10-tetracarboxylic dianhydride
Inchi:	InChI=1S/C24H8O6/c25-21-13-5-1-9-10-2-6-15-20-16(24(28)30-23(15)27)8-4-12(18(10)2
InchiKey:	CLYVDMAATCIVBF-UHFFFAOYSA-N
Formula:	C24H8O6
SMILES:	O=C1OC(=O)c2ccc3c4ccc5c6c(ccc(c7ccc1c2c73)c64)C(=O)OC5=O
Mol. weight [g/mol]:	392.32
CAS:	128-69-8

Physical Properties

Property code	Value	Unit	Source
gf	91.36	kJ/mol	Joback Method
hf	-292.15	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	108.30	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	4.358		Crippen Method
mcvol	248.020	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
tb	1226.28	K	Joback Method
tc	1524.77	K	Joback Method
tf	981.76	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.07	J/mol×K	1226.28	Joback Method
cpg	843.04	J/mol×K	1276.03	Joback Method
cpg	857.37	J/mol×K	1325.78	Joback Method
cpg	872.26	J/mol×K	1375.52	Joback Method
cpg	887.94	J/mol×K	1425.27	Joback Method
cpg	904.61	J/mol×K	1475.02	Joback Method
cpg	922.50	J/mol×K	1524.77	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128698&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

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