3,9-perylenedicarboxylic acid

Inchi: InChI=1S/C22H12O4/c23-21(24)17-9-8-16-12-4-2-6-14-18(22(25)26)10-7-15(20(12)14)1
InchiKey: SDPOODQJUWAHOW-UHFFFAOYSA-N
Formula: C22H12O4
SMILES: O=C(O)c1ccc2c3cccc4c(C(=O)O)ccc(c5cccc1c52)c43
Mol. weight [g/mol]: 340.33
CAS: 6364-19-8

Physical Properties

Property code	Value	Unit	Source
chs	-9741.60	kJ/mol	NIST Webbook
gf	87.98	kJ/mol	Joback Method
hf	-129.03	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	122.93	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	5.134		Crippen Method
mcvol	238.420	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	1114.66	K	Joback Method
tc	1366.51	K	Joback Method
tf	785.30	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.46	J/mol×K	1114.66	Joback Method
cpg	750.90	J/mol×K	1156.64	Joback Method
cpg	766.41	J/mol×K	1198.61	Joback Method
cpg	783.24	J/mol×K	1240.59	Joback Method
cpg	801.62	J/mol×K	1282.56	Joback Method
cpg	821.78	J/mol×K	1324.54	Joback Method
cpg	843.96	J/mol×K	1366.51	Joback Method
dvisc	0.0002568	Pa×s	785.30	Joback Method

dvisc	0.0001756	Pa×s	840.19	Joback Method
dvisc	0.0001258	Pa×s	895.09	Joback Method
dvisc	0.0000936	Pa×s	949.98	Joback Method
dvisc	0.0000720	Pa×s	1004.87	Joback Method
dvisc	0.0000569	Pa×s	1059.77	Joback Method
dvisc	0.0000460	Pa×s	1114.66	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=C6364198&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume