9,10-Phenanthrenedicarboxylic acid, anhydride

Inchi: InChI=1S/C16H8O3/c17-15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16(18)19-15/h1-

InchiKey: RDKMLXMOKXZQMK-UHFFFAOYSA-N

Formula: C16H8O3

SMILES: O=C1OC(=O)c2c1c1ccccc1c1ccccc21

Mol. weight [g/mol]: 248.23

Physical Properties

Property code	Value	Unit	Source
gf	117.82	kJ/mol	Joback Method
hf	-103.57	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	3.304		Crippen Method
mcvol	171.770	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	2598.00		NIST Webbook
tb	819.06	K	Joback Method
tc	1096.69	K	Joback Method
tf	584.65	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.87	J/mol×K	819.06	Joback Method
cpg	495.42	J/mol×K	865.33	Joback Method
cpg	506.94	J/mol×K	911.60	Joback Method
cpg	517.52	J/mol×K	957.88	Joback Method
cpg	527.27	J/mol×K	1004.15	Joback Method
cpg	536.32	J/mol×K	1050.42	Joback Method
cpg	544.76	J/mol×K	1096.69	Joback Method

Sources

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=R553114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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