1,3-DINITROPYRENE

Other names: Pyrene, 1,3-dinitro-
Inchi: InChI=1S/C16H8N2O4/c19-17(20)13-7-6-10-5-4-9-2-1-3-11-14(18(21)22)8-12(13)16(10)
InchiKey: UJIPQBOHUQDIAA-UHFFFAOYSA-N
Formula: C16H8N2O4
SMILES: O=[N+]([O-])c1cc2c([N+](=O)[O-])ccc3ccc4cccc1c4c32
Mol. weight [g/mol]: 292.25

Physical Properties

Property code	Value	Unit	Source
hfus	46.44	kJ/mol	Joback Method
hvap	120.03	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-5.68		Cheméo Relay (1.0)
logp	4.400		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
rinpol	471.19		NIST Webbook
rinpol	471.19		NIST Webbook
tb	722.19	K	Cheméo Relay (1.0)
tf	459.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.72	J/mol×K	965.00	Joback Method
cpg	565.01	J/mol×K	1012.90	Joback Method
cpg	576.59	J/mol×K	1060.79	Joback Method
cpg	588.77	J/mol×K	1108.69	Joback Method
cpg	601.84	J/mol×K	1156.58	Joback Method
cpg	616.09	J/mol×K	1204.48	Joback Method
cpg	631.81	J/mol×K	1252.37	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75321209&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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point