

1,6-Dinitropyrene

Other names:	Pyrene, 1,6-dinitro-
Inchi:	InChI=1S/C16H8N2O4/c19-17(20)13-8-4-10-2-6-12-14(18(21)22)7-3-9-1-5-11(13)16(10)
InchiKey:	GUXACCKTQWVTLG-UHFFFAOYSA-N
Formula:	C16H8N2O4
SMILES:	O=[N+]([O-])c1ccc2ccc3c([N+](=O)[O-])ccc4ccc1c2c43
Mol. weight [g/mol]:	292.25
CAS:	42397-64-8

Physical Properties

Property code	Value	Unit	Source
gf	543.02	kJ/mol	Joback Method
hf	323.31	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	4.400		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	478.51		NIST Webbook
tb	965.00	K	Joback Method
tc	1252.37	K	Joback Method
tf	738.18	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C42397648&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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