1,6-Di-(2,4-dinitro-phenyl)-hexane

Inchi: InChI=1S/C18H18N4O8/c23-19(24)15-9-7-13(17(11-15)21(27)28)5-3-1-2-4-6-14-8-10-16(20(25)26)12-18(14)22(29)30/h7-12H,1-6H2

InchiKey: PQJHKEMRVXUDLF-UHFFFAOYSA-N

Formula: C18H18N4O8

SMILES: O=[N+]([O-])c1ccc(CCCCCCc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])c([N+](=O)[O-])c1

Mol. weight [g/mol]: 418.36

CAS: 6279-98-7

Physical Properties

Property code	Value	Unit	Source
gf	429.18	kJ/mol	Joback Method
hf	-30.71	kJ/mol	Joback Method
hfus	74.35	kJ/mol	Joback Method
hvap	129.23	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	4.665		Crippen Method
mcvol	286.640	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
tb	1291.88	K	Joback Method
tc	1588.46	K	Joback Method
tf	969.98	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.18	J/mol×K	1291.88	Joback Method
cpg	949.64	J/mol×K	1341.31	Joback Method
cpg	955.50	J/mol×K	1390.74	Joback Method
cpg	960.92	J/mol×K	1440.17	Joback Method
cpg	966.08	J/mol×K	1489.60	Joback Method
cpg	971.14	J/mol×K	1539.03	Joback Method
cpg	976.28	J/mol×K	1588.46	Joback Method

Sources

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=C6279987&Units=SI
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
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