Acenaphthene, 5,6-dinitro-

Other names:	Acenaphthylene, 1,2-dihydro-5,6-dinitro- 5,6-Dinitroacenaphthene
Inchi:	InChI=1S/C12H8N2O4/c15-13(16)9-5-3-7-1-2-8-4-6-10(14(17)18)12(9)11(7)8/h3-6H,1-2H
InchiKey:	FIXNUWGGLHPMGU-UHFFFAOYSA-N
Formula:	C12H8N2O4
SMILES:	O=[N+]([O-])c1ccc2c3c(ccc([N+](=O)[O-])c13)CC2
Mol. weight [g/mol]:	244.20
CAS:	4406-87-5

Physical Properties

Property code	Value	Unit	Source
gf	382.36	kJ/mol	Joback Method
hf	168.49	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	2.755		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	850.36	K	Joback Method
tc	1132.28	K	Joback Method
tf	647.12	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.55	J/mol×K	850.36	Joback Method
cpg	459.75	J/mol×K	897.35	Joback Method
cpg	469.48	J/mol×K	944.33	Joback Method
cpg	478.97	J/mol×K	991.32	Joback Method
cpg	488.41	J/mol×K	1038.31	Joback Method
cpg	498.02	J/mol×K	1085.30	Joback Method
cpg	508.01	J/mol×K	1132.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4406875&Units=SI
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

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