Benzene, 1,1'-methylenebis[2-nitro-

Inchi: InChI=1S/C13H10N2O4/c16-14(17)12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)15(18)19/h1-8H
InchiKey: NABSHCGXYOFMDL-UHFFFAOYSA-N
Formula: C13H10N2O4
SMILES: O=[N+]([O-])c1ccccc1Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 258.23
CAS: 21540-57-8

Physical Properties

Property code	Value	Unit	Source
gf	335.24	kJ/mol	Joback Method
hf	116.95	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.094		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	2024.80		NIST Webbook
rinpol	2024.80		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	863.84	K	Joback Method
tc	1147.82	K	Joback Method
tf	601.37	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.84	J/mol×K	863.84	Joback Method
cpg	521.82	J/mol×K	911.17	Joback Method
cpg	531.63	J/mol×K	958.50	Joback Method
cpg	540.36	J/mol×K	1005.83	Joback Method
cpg	548.15	J/mol×K	1053.16	Joback Method

cpg	555.09	J/mol×K	1100.49	Joback Method
cpg	561.33	J/mol×K	1147.82	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=C21540578&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume