Diphenylmethane, 2,4-dinitro

Inchi: InChI=1S/C13H10N2O4/c16-14(17)12-7-11(8-13(9-12)15(18)19)6-10-4-2-1-3-5-10/h1-5,7
InchiKey: IDEMWJLVAXXOGJ-UHFFFAOYSA-N
Formula: C13H10N2O4
SMILES: O=[N+]([O-])c1cc(Cc2ccccc2)cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 258.23

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	2209.00		NIST Webbook
rinpol	2118.30		NIST Webbook
rinpol	2118.30		NIST Webbook
rinpol	2209.00		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

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=R237515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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