P-toluenesulfonamide, n-(2,4-dinitro-1-naphthyl)-

Inchi: InChI=1S/C17H13N3O6S/c1-11-6-8-12(9-7-11)27(25,26)18-17-14-5-3-2-4-13(14)15(19(2

InchiKey: JSEQBQKZIDGOBK-UHFFFAOYSA-N

Formula: C17H13N3O6S

SMILES: Cc1ccc(S(=O)(=O)Nc2c([N+](=O)[O-])cc([N+](=O)[O-])c3ccccc23)cc1

Mol. weight [g/mol]: 387.37

CAS: 52077-96-0

Physical Properties

Property code	Value	Unit	Source
gf	77.16	kJ/mol	Joback Method
hf	-197.36	kJ/mol	Joback Method
hfus	62.53	kJ/mol	Joback Method
hvap	120.53	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	3.765		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	1082.25	K	Joback Method
tc	1356.19	K	Joback Method
tf	795.41	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.53	J/mol×K	1082.25	Joback Method
cpg	777.44	J/mol×K	1127.91	Joback Method
cpg	783.27	J/mol×K	1173.56	Joback Method
cpg	788.14	J/mol×K	1219.22	Joback Method
cpg	792.16	J/mol×K	1264.87	Joback Method
cpg	795.47	J/mol×K	1310.53	Joback Method
cpg	798.17	J/mol×K	1356.19	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=C52077960&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume