

Benzene, 1-(2-methylphenoxy)-2,4-dinitro-

Other names:

Ether, 2,4-dinitrophenyl o-tolyl
o-Tolyl 2,4-dinitrophenyl ether
2,4-Dinitrophenyl o-tolyl ether
2,4-Dinitro-2'-methyl-diphenyl ether
2,4-Dinitrophenyl 2-methylphenyl ether

Inchi:

InChI=1S/C13H10N2O5/c1-9-4-2-3-5-12(9)20-13-7-6-10(14(16)17)8-11(13)15(18)19/h2-

InchiKey:

NYOFYDDSVHVPEM-UHFFFAOYSA-N

Formula:

C13H10N2O5

SMILES:

Cc1ccccc1Oc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]

Mol. weight [g/mol]:

274.23

CAS:

2363-26-0

Physical Properties

Property code	Value	Unit	Source
gf	220.61	kJ/mol	Joback Method
hf	-26.74	kJ/mol	Joback Method
hfus	40.25	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.604		Crippen Method
mcvol	187.220	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpola	371.07		NIST Webbook
tb	891.24	K	Joback Method
tc	1170.47	K	Joback Method
tf	636.12	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.81	J/molxK	891.24	Joback Method
cpg	543.07	J/molxK	937.78	Joback Method
cpg	552.05	J/molxK	984.32	Joback Method

cpg	559.81	J/mol×K	1030.85	Joback Method
cpg	566.42	J/mol×K	1077.39	Joback Method
cpg	571.93	J/mol×K	1123.93	Joback Method
cpg	576.41	J/mol×K	1170.47	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=C2363260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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