

(2E)-1,3-bis(3-nitrophenyl)-2-buten-1-one

Inchi:	InChI=1S/C16H12N2O5/c1-11(12-4-2-6-14(9-12)17(20)21)8-16(19)13-5-3-7-15(10-13)18
InchiKey:	HYANPVXC�XDNLW-DHZHZOJOSA-N
Formula:	C16H12N2O5
SMILES:	CC(=CC(=O)c1cccc([N+](=O)[O-])c1)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	312.28
CAS:	7509-22-0

Physical Properties

Property code	Value	Unit	Source
gf	303.25	kJ/mol	Joback Method
hf	49.88	kJ/mol	Joback Method
hfus	47.71	kJ/mol	Joback Method
hvap	97.05	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	3.789		Crippen Method
mcvol	220.890	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	990.39	K	Joback Method
tc	1272.10	K	Joback Method
tf	666.07	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.15	J/molxK	990.39	Joback Method
cpg	660.20	J/molxK	1037.34	Joback Method
cpg	669.42	J/molxK	1084.29	Joback Method
cpg	677.96	J/molxK	1131.25	Joback Method
cpg	685.99	J/molxK	1178.20	Joback Method
cpg	693.67	J/molxK	1225.15	Joback Method
cpg	701.16	J/molxK	1272.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7509220&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

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