2'-Methyl-3',5'-dinitro-chalcone

Inchi: InChI=1S/C16H12N2O5/c1-11-14(9-13(17(20)21)10-15(11)18(22)23)16(19)8-7-12-5-3-2-
InchiKey: LJAPVXYKCUGLLE-BQYQJAHWSA-N
Formula: C16H12N2O5
SMILES: Cc1c(C(=O)C=Cc2ccccc2)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 312.28
CAS: 5333-00-6

Physical Properties

Property code	Value	Unit	Source
gf	302.17	kJ/mol	Joback Method
hf	48.20	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	97.63	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	3.708		Crippen Method
mcvol	220.890	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
tb	995.49	K	Joback Method
tc	1274.07	K	Joback Method
tf	692.55	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.52	J/mol×K	995.49	Joback Method
cpg	658.31	J/mol×K	1041.92	Joback Method
cpg	667.23	J/mol×K	1088.35	Joback Method
cpg	675.44	J/mol×K	1134.78	Joback Method
cpg	683.06	J/mol×K	1181.21	Joback Method
cpg	690.24	J/mol×K	1227.64	Joback Method
cpg	697.12	J/mol×K	1274.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5333006&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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