Methyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro-, methyl ester
Inchi: InChI=1S/C8H6N2O6/c1-16-8(11)5-2-6(9(12)13)4-7(3-5)10(14)15/h2-4H,1H3
InchiKey: POGCCFLNFPIIGW-UHFFFAOYSA-N
Formula: C8H6N2O6
SMILES: COC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 226.14
CAS: 2702-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-53.19	kJ/mol	Joback Method
hf	-261.18	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.290		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
ripol	2729.00		NIST Webbook
ripol	2762.00		NIST Webbook
ripol	2780.00		NIST Webbook
ripol	2749.00		NIST Webbook
ripol	2729.00		NIST Webbook
tb	799.05	K	Joback Method
tc	1065.57	K	Joback Method
tf	590.76	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.07	J/mol×K	799.05	Joback Method
cpg	384.68	J/mol×K	843.47	Joback Method
cpg	392.33	J/mol×K	887.89	Joback Method
cpg	399.02	J/mol×K	932.31	Joback Method
cpg	404.78	J/mol×K	976.73	Joback Method
cpg	409.62	J/mol×K	1021.15	Joback Method
cpg	413.57	J/mol×K	1065.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2702581&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume