Ethyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro-, ethyl ester
Inchi: InChI=1S/C9H8N2O6/c1-2-17-9(12)6-3-7(10(13)14)5-8(4-6)11(15)16/h3-5H,2H2,1H3
InchiKey: IBQREHJPMPCXQA-UHFFFAOYSA-N
Formula: C9H8N2O6
SMILES: CCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 240.17
CAS: 618-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-44.77	kJ/mol	Joback Method
hf	-281.82	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	1.680		Crippen Method
mcvol	156.190	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1810.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2792.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2749.00		NIST Webbook
ripol	2753.00		NIST Webbook

ripol	2792.00		NIST Webbook
ripol	2774.00		NIST Webbook
ripol	2753.00		NIST Webbook
ripol	2781.00		NIST Webbook
ripol	2764.00		NIST Webbook
tb	821.93	K	Joback Method
tc	1082.48	K	Joback Method
tf	602.03	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.66	J/mol×K	821.93	Joback Method
cpg	436.84	J/mol×K	865.36	Joback Method
cpg	445.02	J/mol×K	908.78	Joback Method
cpg	452.21	J/mol×K	952.21	Joback Method
cpg	458.45	J/mol×K	995.63	Joback Method
cpg	463.74	J/mol×K	1039.06	Joback Method
cpg	468.12	J/mol×K	1082.48	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618713&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