Benzoic acid, 3,5-dinitro, isopropyl ester

Other names: Benzoic acid, 3,5-dinitro, 1-methylethyl ester
Inchi: InChI=1S/C10H10N2O6/c1-6(2)18-10(13)7-3-8(11(14)15)5-9(4-7)12(16)17/h3-6H,1-2H3
InchiKey: FAYNAMQMBONHIQ-UHFFFAOYSA-N
Formula: C10H10N2O6
SMILES: CC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 254.20
CAS: 10477-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-38.79	kJ/mol	Joback Method
hf	-307.74	kJ/mol	Joback Method
hfus	36.90	kJ/mol	Joback Method
hvap	83.40	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	2.068		Crippen Method
mcvol	170.280	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2759.00		NIST Webbook
ripol	2746.00		NIST Webbook
ripol	2738.00		NIST Webbook
ripol	2746.00		NIST Webbook
ripol	2781.00		NIST Webbook
ripol	2738.00		NIST Webbook
tb	844.37	K	Joback Method
tc	1104.14	K	Joback Method
tf	598.30	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.95	J/mol×K	844.37	Joback Method
cpg	490.75	J/mol×K	887.66	Joback Method
cpg	499.45	J/mol×K	930.96	Joback Method
cpg	507.10	J/mol×K	974.25	Joback Method
cpg	513.71	J/mol×K	1017.55	Joback Method
cpg	519.31	J/mol×K	1060.84	Joback Method
cpg	523.94	J/mol×K	1104.14	Joback Method

Sources

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=C10477993&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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