Benzoic acid, 3,5-dinitro, 1-methylethyl 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

Physical Properties

Property code	Value	Unit	Source
hf	-331.97	kJ/mol	Cheméo Relay (1.0)
hfus	36.90	kJ/mol	Joback Method
hvap	87.46	kJ/mol	Cheméo Relay (1.0)
ie	10.32	eV	Cheméo Relay (1.0)
log10ws	-3.45		Cheméo Relay (1.0)
logp	2.068		Crippen Method
mcvol	170.280	ml/mol	McGowan Method
rinpol	1788.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2781.00		NIST Webbook
ripol	2746.00		NIST Webbook
ripol	2738.00		NIST Webbook
ripol	2746.00		NIST Webbook
ripol	2759.00		NIST Webbook
ripol	2738.00		NIST Webbook
tb	562.99	K	Cheméo Relay (1.0)
tf	341.25	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10477993&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point