propyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C10H10N2O6/c1-2-3-18-10(13)7-4-8(11(14)15)6-9(5-7)12(16)17/h4-6H,2-3H2,
InchiKey: DAUPVRJTSBTYTP-UHFFFAOYSA-N
Formula: C10H10N2O6
SMILES: CCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 254.20
CAS: 10478-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.35	kJ/mol	Joback Method
hf	-302.46	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	83.79	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.070		Crippen Method
mcvol	170.280	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
ripol	2826.00		NIST Webbook
ripol	2784.00		NIST Webbook
ripol	2809.00		NIST Webbook
ripol	2803.00		NIST Webbook
ripol	2784.00		NIST Webbook
ripol	2803.00		NIST Webbook
tb	844.81	K	Joback Method
tc	1100.00	K	Joback Method
tf	613.30	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.32	J/mol×K	844.81	Joback Method
cpg	489.98	J/mol×K	887.34	Joback Method
cpg	498.59	J/mol×K	929.87	Joback Method
cpg	506.20	J/mol×K	972.40	Joback Method
cpg	512.83	J/mol×K	1014.94	Joback Method
cpg	518.50	J/mol×K	1057.47	Joback Method
cpg	523.24	J/mol×K	1100.00	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10478009&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