Benzoic acid, 3,5-dinitro, 1-methylpropyl ester

Inchi: InChI=1S/C11H12N2O6/c1-3-7(2)19-11(14)8-4-9(12(15)16)6-10(5-8)13(17)18/h4-7H,3H2
InchiKey: SWFWVZZGOVUDMH-UHFFFAOYSA-N
Formula: C11H12N2O6
SMILES: CCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 268.22
CAS: 7510-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-30.37	kJ/mol	Joback Method
hf	-328.38	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	2.458		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1872.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1872.00		NIST Webbook
ripol	2748.00		NIST Webbook
ripol	2757.00		NIST Webbook
ripol	2748.00		NIST Webbook
ripol	2764.00		NIST Webbook
ripol	2785.00		NIST Webbook
ripol	2757.00		NIST Webbook
tb	867.25	K	Joback Method
tc	1121.93	K	Joback Method
tf	609.57	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.59	J/mol×K	867.25	Joback Method
cpg	544.76	J/mol×K	909.70	Joback Method
cpg	553.82	J/mol×K	952.14	Joback Method
cpg	561.80	J/mol×K	994.59	Joback Method
cpg	568.73	J/mol×K	1037.04	Joback Method
cpg	574.64	J/mol×K	1079.48	Joback Method
cpg	579.57	J/mol×K	1121.93	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=C7510578&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