pentyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C12H14N2O6/c1-2-3-4-5-20-12(15)9-6-10(13(16)17)8-11(7-9)14(18)19/h6-8H,
InchiKey: KVRKVNNGYVWNGH-UHFFFAOYSA-N
Formula: C12H14N2O6
SMILES: CCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 282.25
CAS: 10478-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-19.51	kJ/mol	Joback Method
hf	-343.74	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	88.24	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	2.850		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2074.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2058.00		NIST Webbook
ripol	2969.00		NIST Webbook
ripol	2969.00		NIST Webbook
ripol	3007.00		NIST Webbook
ripol	3007.00		NIST Webbook
ripol	3007.00		NIST Webbook
ripol	2993.00		NIST Webbook
tb	890.57	K	Joback Method
tc	1136.97	K	Joback Method
tf	635.84	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.58	J/mol×K	890.57	Joback Method
cpg	598.94	J/mol×K	931.64	Joback Method
cpg	608.21	J/mol×K	972.70	Joback Method
cpg	616.44	J/mol×K	1013.77	Joback Method
cpg	623.65	J/mol×K	1054.84	Joback Method
cpg	629.89	J/mol×K	1095.91	Joback Method
cpg	635.17	J/mol×K	1136.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10478032&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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