Pentan-2-yl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, 1-methylbutyl ester
Inchi: InChI=1S/C12H14N2O6/c1-3-4-8(2)20-12(15)9-5-10(13(16)17)7-11(6-9)14(18)19/h5-8H,
InchiKey: UJIRDPTTWKRINN-UHFFFAOYSA-N
Formula: C12H14N2O6
SMILES: CCCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 282.25

Physical Properties

Property code	Value	Unit	Source
gf	-21.95	kJ/mol	Joback Method
hf	-349.02	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	87.86	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	2.848		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1971.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
ripol	2835.00		NIST Webbook
ripol	2835.00		NIST Webbook
ripol	2818.00		NIST Webbook
ripol	2834.00		NIST Webbook
ripol	2855.00		NIST Webbook
ripol	2818.00		NIST Webbook
tb	890.13	K	Joback Method
tc	1140.38	K	Joback Method
tf	620.84	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.16	J/mol×K	890.13	Joback Method
cpg	599.63	J/mol×K	931.84	Joback Method
cpg	608.98	J/mol×K	973.55	Joback Method
cpg	617.22	J/mol×K	1015.26	Joback Method
cpg	624.41	J/mol×K	1056.96	Joback Method
cpg	630.57	J/mol×K	1098.67	Joback Method
cpg	635.74	J/mol×K	1140.38	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373868&Units=SI

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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