hexyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C13H16N2O6/c1-2-3-4-5-6-21-13(16)10-7-11(14(17)18)9-12(8-10)15(19)20/h7
InchiKey: KZVBOYCZXPUDGJ-UHFFFAOYSA-N
Formula: C13H16N2O6
SMILES: CCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 296.28
CAS: 10478-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-11.09	kJ/mol	Joback Method
hf	-364.38	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	90.47	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.240		Crippen Method
mcvol	212.550	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	2173.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2162.00		NIST Webbook
ripol	3089.00		NIST Webbook
ripol	3103.00		NIST Webbook
ripol	3108.00		NIST Webbook
ripol	3067.00		NIST Webbook
tb	913.45	K	Joback Method
tc	1156.49	K	Joback Method
tf	647.11	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.03	J/mol×K	913.45	Joback Method
cpg	654.65	J/mol×K	953.96	Joback Method
cpg	664.17	J/mol×K	994.46	Joback Method
cpg	672.62	J/mol×K	1034.97	Joback Method
cpg	680.05	J/mol×K	1075.48	Joback Method
cpg	686.49	J/mol×K	1115.99	Joback Method
cpg	691.97	J/mol×K	1156.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10478043&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