2-Cyclohexyl-4,6-dinitrophenyl propionate

Inchi: InChI=1S/C15H18N2O6/c1-2-14(18)23-15-12(10-6-4-3-5-7-10)8-11(16(19)20)9-13(15)17
InchiKey: YERJOKQGQHMPIO-UHFFFAOYSA-N
Formula: C15H18N2O6
SMILES: CCC(=O)Oc1c(C2CCCCC2)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 322.31
CAS: 116632-95-2

Physical Properties

Property code	Value	Unit	Source
gf	20.57	kJ/mol	Joback Method
hf	-362.81	kJ/mol	Joback Method
hfus	44.82	kJ/mol	Joback Method
hvap	96.01	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	3.866		Crippen Method
mcvol	229.870	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
tb	983.74	K	Joback Method
tc	1249.36	K	Joback Method
tf	689.55	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.41	J/mol×K	983.74	Joback Method
cpg	757.29	J/mol×K	1028.01	Joback Method
cpg	766.56	J/mol×K	1072.28	Joback Method
cpg	774.27	J/mol×K	1116.55	Joback Method
cpg	780.48	J/mol×K	1160.82	Joback Method
cpg	785.24	J/mol×K	1205.09	Joback Method
cpg	788.59	J/mol×K	1249.36	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=C116632952&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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