1,1'-Oxy-di-2-propanol di-p-nitro benzoate

Inchi: InChI=1S/C20H20N2O9/c1-13(30-19(23)15-3-7-17(8-4-15)21(25)26)11-29-12-14(2)31-20
InchiKey: ZWENNPIYTJYTCZ-UHFFFAOYSA-N
Formula: C20H20N2O9
SMILES: CC(COCC(C)OC(=O)c1ccc([N+](=O)[O-])cc1)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 432.38
CAS: 95429-50-8

Physical Properties

Property code	Value	Unit	Source
gf	-183.54	kJ/mol	Joback Method
hf	-659.91	kJ/mol	Joback Method
hfus	57.30	kJ/mol	Joback Method
hvap	119.12	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	3.310		Crippen Method
mcvol	300.730	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
tb	1198.12	K	Joback Method
tc	1470.83	K	Joback Method
tf	816.81	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.05	J/mol×K	1198.12	Joback Method
cpg	971.35	J/mol×K	1243.57	Joback Method
cpg	971.70	J/mol×K	1289.02	Joback Method
cpg	970.15	J/mol×K	1334.47	Joback Method
cpg	966.75	J/mol×K	1379.93	Joback Method
cpg	961.55	J/mol×K	1425.38	Joback Method
cpg	954.58	J/mol×K	1470.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95429508&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

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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