3-Phenoxybenzyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C20H14N2O7/c23-20(15-10-16(21(24)25)12-17(11-15)22(26)27)28-13-14-5-4-
InchiKey: BUHSFUZRXFWOLT-UHFFFAOYSA-N
Formula: C20H14N2O7
SMILES: O=C(OCc1cccc(Oc2ccccc2)c1)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 394.33

Physical Properties

Property code	Value	Unit	Source
gf	158.04	kJ/mol	Joback Method
hf	-179.49	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	113.68	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	4.652		Crippen Method
mcvol	269.530	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	3189.00		NIST Webbook
rinpol	3189.00		NIST Webbook
tb	1154.37	K	Joback Method
tc	1438.81	K	Joback Method
tf	813.59	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.81	J/mol×K	1154.37	Joback Method
cpg	836.52	J/mol×K	1201.78	Joback Method
cpg	839.73	J/mol×K	1249.18	Joback Method
cpg	841.53	J/mol×K	1296.59	Joback Method
cpg	842.03	J/mol×K	1344.00	Joback Method
cpg	841.32	J/mol×K	1391.40	Joback Method
cpg	839.48	J/mol×K	1438.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373879&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume