Pimelic acid, di(2-nitro-5-fluorophenyl) ester

Inchi: InChI=1S/C19H16F2N2O8/c20-12-6-8-14(22(26)27)16(10-12)30-18(24)4-2-1-3-5-19(25)3
InchiKey: BZJCYBZGPKLWBO-UHFFFAOYSA-N
Formula: C19H16F2N2O8
SMILES: O=C(CCCCCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])Oc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 438.34

Physical Properties

Property code	Value	Unit	Source
gf	-490.96	kJ/mol	Joback Method
hf	-911.65	kJ/mol	Joback Method
hfus	65.95	kJ/mol	Joback Method
hvap	114.95	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	4.243		Crippen Method
mcvol	284.310	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	1162.20	K	Joback Method
tc	1424.85	K	Joback Method
tf	839.53	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.10	J/mol×K	1162.20	Joback Method
cpg	905.05	J/mol×K	1205.98	Joback Method
cpg	907.42	J/mol×K	1249.75	Joback Method
cpg	908.27	J/mol×K	1293.53	Joback Method
cpg	907.64	J/mol×K	1337.30	Joback Method
cpg	905.56	J/mol×K	1381.08	Joback Method
cpg	902.09	J/mol×K	1424.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416481&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