Pimelic acid, 2-nitro-5-fluorophenyl octyl ester

Inchi: InChI=1S/C21H30FNO6/c1-2-3-4-5-6-10-15-28-20(24)11-8-7-9-12-21(25)29-19-16-17(22
InchiKey: OJXZPCDVDZBREW-UHFFFAOYSA-N
Formula: C21H30FNO6
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)Oc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 411.46

Physical Properties

Property code	Value	Unit	Source
gf	-408.01	kJ/mol	Joback Method
hf	-959.65	kJ/mol	Joback Method
hfus	63.42	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	5.493		Crippen Method
mcvol	317.060	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2946.00		NIST Webbook
rinpol	2946.00		NIST Webbook
tb	1020.21	K	Joback Method
tc	1249.17	K	Joback Method
tf	666.41	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.62	J/mol×K	1020.21	Joback Method
cpg	1065.98	J/mol×K	1058.37	Joback Method
cpg	1076.89	J/mol×K	1096.53	Joback Method
cpg	1086.41	J/mol×K	1134.69	Joback Method
cpg	1094.55	J/mol×K	1172.85	Joback Method
cpg	1101.37	J/mol×K	1211.01	Joback Method
cpg	1106.89	J/mol×K	1249.17	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=U416479&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume