Pimelic acid, 4-methyl-2-pentyl 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C19H26FNO6/c1-13(2)11-14(3)26-18(22)7-5-4-6-8-19(23)27-17-12-15(20)9-10

InchiKey: QPUZXBKCEMQSEN-UHFFFAOYSA-N

Formula: C19H26FNO6

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)Oc1cc(F)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 383.41

Physical Properties

Property code	Value	Unit	Source
gf	-429.73	kJ/mol	Joback Method
hf	-928.93	kJ/mol	Joback Method
hfus	51.20	kJ/mol	Joback Method
hvap	94.80	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.568		Crippen Method
mcvol	288.880	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	973.57	K	Joback Method
tc	1197.58	K	Joback Method
tf	613.87	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.67	J/mol×K	973.57	Joback Method
cpg	947.75	J/mol×K	1010.90	Joback Method
cpg	958.49	J/mol×K	1048.24	Joback Method
cpg	967.90	J/mol×K	1085.57	Joback Method
cpg	976.02	J/mol×K	1122.91	Joback Method
cpg	982.87	J/mol×K	1160.24	Joback Method
cpg	988.48	J/mol×K	1197.58	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=U416475&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