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

Inchi: InChI=1S/C18H24FNO6/c1-2-3-7-12-25-17(21)8-5-4-6-9-18(22)26-16-13-14(19)10-11-15

InchiKey: GHYGYEPVQJMJGP-UHFFFAOYSA-N

Formula: C18H24FNO6

SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1cc(F)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 369.38

Physical Properties

Property code	Value	Unit	Source
gf	-433.27	kJ/mol	Joback Method
hf	-897.73	kJ/mol	Joback Method
hfus	55.65	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.323		Crippen Method
mcvol	274.790	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2641.00		NIST Webbook
rinpol	2641.00		NIST Webbook
tb	951.57	K	Joback Method
tc	1171.31	K	Joback Method
tf	632.60	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.18	J/mol×K	951.57	Joback Method
cpg	888.12	J/mol×K	988.19	Joback Method
cpg	898.82	J/mol×K	1024.82	Joback Method
cpg	908.30	J/mol×K	1061.44	Joback Method
cpg	916.59	J/mol×K	1098.06	Joback Method
cpg	923.72	J/mol×K	1134.69	Joback Method
cpg	929.69	J/mol×K	1171.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416476&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