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

Inchi: InChI=1S/C16H20FNO6/c1-2-10-23-15(19)6-4-3-5-7-16(20)24-14-11-12(17)8-9-13(14)18

InchiKey: HPDIIJZPQXHANU-UHFFFAOYSA-N

Formula: C16H20FNO6

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

Mol. weight [g/mol]: 341.33

Physical Properties

Property code	Value	Unit	Source
gf	-450.11	kJ/mol	Joback Method
hf	-856.45	kJ/mol	Joback Method
hfus	50.47	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.543		Crippen Method
mcvol	246.610	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	905.81	K	Joback Method
tc	1123.91	K	Joback Method
tf	610.06	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.78	J/mol×K	905.81	Joback Method
cpg	772.39	J/mol×K	942.16	Joback Method
cpg	782.86	J/mol×K	978.51	Joback Method
cpg	792.20	J/mol×K	1014.86	Joback Method
cpg	800.44	J/mol×K	1051.21	Joback Method
cpg	807.59	J/mol×K	1087.56	Joback Method
cpg	813.66	J/mol×K	1123.91	Joback Method

Sources

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=U416472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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