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

Inchi: InChI=1S/C17H22FNO6/c1-12(2)11-24-16(20)6-4-3-5-7-17(21)25-15-10-13(18)8-9-14(15

InchiKey: WNGYFRHSMGNKDU-UHFFFAOYSA-N

Formula: C17H22FNO6

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

Mol. weight [g/mol]: 355.36

Physical Properties

Property code	Value	Unit	Source
gf	-444.13	kJ/mol	Joback Method
hf	-882.37	kJ/mol	Joback Method
hfus	49.54	kJ/mol	Joback Method
hvap	90.73	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.789		Crippen Method
mcvol	260.700	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	928.25	K	Joback Method
tc	1148.50	K	Joback Method
tf	606.33	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.66	J/mol×K	928.25	Joback Method
cpg	830.49	J/mol×K	964.96	Joback Method
cpg	841.10	J/mol×K	1001.67	Joback Method
cpg	850.52	J/mol×K	1038.37	Joback Method
cpg	858.76	J/mol×K	1075.08	Joback Method
cpg	865.83	J/mol×K	1111.79	Joback Method
cpg	871.77	J/mol×K	1148.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416473&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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