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

Inchi: InChI=1S/C20H28FNO6/c1-2-3-4-5-9-14-27-19(23)10-7-6-8-11-20(24)28-18-15-16(21)12

InchiKey: GAAISMLRPVVQRW-UHFFFAOYSA-N

Formula: C20H28FNO6

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

Mol. weight [g/mol]: 397.44

Physical Properties

Property code	Value	Unit	Source
gf	-416.43	kJ/mol	Joback Method
hf	-939.01	kJ/mol	Joback Method
hfus	60.83	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.103		Crippen Method
mcvol	302.970	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	997.33	K	Joback Method
tc	1222.24	K	Joback Method
tf	655.14	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.96	J/mol×K	997.33	Joback Method
cpg	1006.19	J/mol×K	1034.81	Joback Method
cpg	1017.04	J/mol×K	1072.30	Joback Method
cpg	1026.57	J/mol×K	1109.78	Joback Method
cpg	1034.79	J/mol×K	1147.27	Joback Method
cpg	1041.75	J/mol×K	1184.75	Joback Method
cpg	1047.46	J/mol×K	1222.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416478&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