5-Phenylvaleric acid, 4-nitrophenyl ester

Inchi: InChI=1S/C17H17NO4/c19-17(9-5-4-8-14-6-2-1-3-7-14)22-16-12-10-15(11-13-16)18(20)
InchiKey: ZYOACALDCIBHLM-UHFFFAOYSA-N
Formula: C17H17NO4
SMILES: O=C(CCCCc1ccccc1)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
gf	109.08	kJ/mol	Joback Method
hf	-188.18	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	84.40	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.913		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	874.83	K	Joback Method
tc	1121.49	K	Joback Method
tf	562.48	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.68	J/mol×K	874.83	Joback Method
cpg	687.54	J/mol×K	915.94	Joback Method
cpg	699.15	J/mol×K	957.05	Joback Method
cpg	709.59	J/mol×K	998.16	Joback Method
cpg	718.93	J/mol×K	1039.27	Joback Method
cpg	727.23	J/mol×K	1080.38	Joback Method
cpg	734.58	J/mol×K	1121.49	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=U406901&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