Sarcosine, N-(4-nitrobenzoyl)-, pentyl ester

Inchi: InChI=1S/C15H20N2O5/c1-3-4-5-10-22-14(18)11-16(2)15(19)12-6-8-13(9-7-12)17(20)21
InchiKey: GQKQRBUEHNOZJK-UHFFFAOYSA-N
Formula: C15H20N2O5
SMILES: CCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-38.31	kJ/mol	Joback Method
hf	-428.48	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.400		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	868.70	K	Joback Method
tc	1091.63	K	Joback Method
tf	595.92	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.93	J/mol×K	868.70	Joback Method
cpg	725.42	J/mol×K	905.86	Joback Method
cpg	736.85	J/mol×K	943.01	Joback Method
cpg	747.27	J/mol×K	980.17	Joback Method
cpg	756.71	J/mol×K	1017.32	Joback Method
cpg	765.23	J/mol×K	1054.48	Joback Method
cpg	772.87	J/mol×K	1091.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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