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

Inchi: InChI=1S/C12H14N2O5/c1-3-19-11(15)8-13(2)12(16)9-4-6-10(7-5-9)14(17)18/h4-7H,3,8
InchiKey: HRCVPDCQBGOHDU-UHFFFAOYSA-N
Formula: C12H14N2O5
SMILES: CCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 266.25

Physical Properties

Property code	Value	Unit	Source
gf	-63.57	kJ/mol	Joback Method
hf	-366.56	kJ/mol	Joback Method
hfus	39.26	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.230		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	800.06	K	Joback Method
tc	1030.84	K	Joback Method
tf	562.11	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.78	J/mol×K	800.06	Joback Method
cpg	559.42	J/mol×K	838.52	Joback Method
cpg	570.03	J/mol×K	876.99	Joback Method
cpg	579.68	J/mol×K	915.45	Joback Method
cpg	588.39	J/mol×K	953.91	Joback Method
cpg	596.21	J/mol×K	992.38	Joback Method
cpg	603.17	J/mol×K	1030.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321280&Units=SI

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