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

Inchi: InChI=1S/C14H18N2O5/c1-3-4-9-21-13(17)10-15(2)14(18)11-5-7-12(8-6-11)16(19)20/h5
InchiKey: HZBPUXWDEZNLPF-UHFFFAOYSA-N
Formula: C14H18N2O5
SMILES: CCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
gf	-46.73	kJ/mol	Joback Method
hf	-407.84	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.010		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	845.82	K	Joback Method
tc	1070.74	K	Joback Method
tf	584.65	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.96	J/mol×K	845.82	Joback Method
cpg	669.21	J/mol×K	883.31	Joback Method
cpg	680.41	J/mol×K	920.79	Joback Method
cpg	690.61	J/mol×K	958.28	Joback Method
cpg	699.85	J/mol×K	995.76	Joback Method
cpg	708.17	J/mol×K	1033.25	Joback Method
cpg	715.63	J/mol×K	1070.74	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=U321283&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