Sarcosine, N-(4-nitrobenzoyl-, propyl ester

Inchi: InChI=1S/C13H16N2O5/c1-3-8-20-12(16)9-14(2)13(17)10-4-6-11(7-5-10)15(18)19/h4-7H
InchiKey: JDTAJJRQJXNIJX-UHFFFAOYSA-N
Formula: C13H16N2O5
SMILES: CCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 280.28

Physical Properties

Property code	Value	Unit	Source
gf	-55.15	kJ/mol	Joback Method
hf	-387.20	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	82.01	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.620		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	822.94	K	Joback Method
tc	1050.49	K	Joback Method
tf	573.38	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.89	J/mol×K	822.94	Joback Method
cpg	613.85	J/mol×K	860.86	Joback Method
cpg	624.79	J/mol×K	898.79	Joback Method
cpg	634.73	J/mol×K	936.71	Joback Method
cpg	643.73	J/mol×K	974.64	Joback Method
cpg	651.83	J/mol×K	1012.56	Joback Method
cpg	659.06	J/mol×K	1050.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321281&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