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

Inchi: InChI=1S/C16H22N2O5/c1-3-4-5-6-11-23-15(19)12-17(2)16(20)13-7-9-14(10-8-13)18(21
InchiKey: PYUHYYKSGMOBEY-UHFFFAOYSA-N
Formula: C16H22N2O5
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 322.36

Physical Properties

Property code	Value	Unit	Source
gf	-29.89	kJ/mol	Joback Method
hf	-449.12	kJ/mol	Joback Method
hfus	49.62	kJ/mol	Joback Method
hvap	88.68	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.790		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	891.58	K	Joback Method
tc	1113.22	K	Joback Method
tf	607.19	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.73	J/mol×K	891.58	Joback Method
cpg	782.44	J/mol×K	928.52	Joback Method
cpg	794.07	J/mol×K	965.46	Joback Method
cpg	804.67	J/mol×K	1002.40	Joback Method
cpg	814.29	J/mol×K	1039.34	Joback Method
cpg	822.98	J/mol×K	1076.28	Joback Method
cpg	830.78	J/mol×K	1113.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321285&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