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

Inchi: InChI=1S/C18H26N2O5/c1-3-4-5-6-7-8-13-25-17(21)14-19(2)18(22)15-9-11-16(12-10-15
InchiKey: QEURJEZPYYPEEO-UHFFFAOYSA-N
Formula: C18H26N2O5
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-13.05	kJ/mol	Joback Method
hf	-490.40	kJ/mol	Joback Method
hfus	54.80	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.571		Crippen Method
mcvol	277.130	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2853.00		NIST Webbook
tb	937.34	K	Joback Method
tc	1158.63	K	Joback Method
tf	629.73	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.60	J/mol×K	937.34	Joback Method
cpg	898.71	J/mol×K	974.22	Joback Method
cpg	910.69	J/mol×K	1011.10	Joback Method
cpg	921.61	J/mol×K	1047.98	Joback Method
cpg	931.51	J/mol×K	1084.86	Joback Method
cpg	940.46	J/mol×K	1121.75	Joback Method
cpg	948.52	J/mol×K	1158.63	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=U321287&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