Sarcosine, N-(3-methoxybenzoyl)-, undecyl ester

Inchi: InChI=1S/C22H35NO4/c1-4-5-6-7-8-9-10-11-12-16-27-21(24)18-23(2)22(25)19-14-13-15

InchiKey: REJCNXBKRGKSPL-UHFFFAOYSA-N

Formula: C22H35NO4

SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1

Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
gf	-119.92	kJ/mol	Joback Method
hf	-694.42	kJ/mol	Joback Method
hfus	54.98	kJ/mol	Joback Method
hvap	87.86	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.841		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1169.62	kPa	Joback Method
rinpol	3001.00		NIST Webbook
tb	899.44	K	Joback Method
tc	1103.83	K	Joback Method
tf	553.43	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.41	J/mol×K	899.44	Joback Method
cpg	1057.01	J/mol×K	933.51	Joback Method
cpg	1072.35	J/mol×K	967.57	Joback Method
cpg	1086.48	J/mol×K	1001.64	Joback Method
cpg	1099.44	J/mol×K	1035.70	Joback Method
cpg	1111.25	J/mol×K	1069.77	Joback Method
cpg	1121.97	J/mol×K	1103.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321499&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

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