Sarcosine, N-(2-methoxybenzoyl)-, dodecyl ester

Inchi: InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-15-18-28-22(25)19-24(2)23(26)20-16-13

InchiKey: WBUHIEWJIOOIIY-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1OC

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
gf	-111.50	kJ/mol	Joback Method
hf	-715.06	kJ/mol	Joback Method
hfus	57.57	kJ/mol	Joback Method
hvap	90.08	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.231		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	922.32	K	Joback Method
tc	1130.08	K	Joback Method
tf	564.70	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.47	J/mol×K	922.32	Joback Method
cpg	1118.31	J/mol×K	956.95	Joback Method
cpg	1133.84	J/mol×K	991.57	Joback Method
cpg	1148.09	J/mol×K	1026.20	Joback Method
cpg	1161.12	J/mol×K	1060.83	Joback Method
cpg	1172.95	J/mol×K	1095.45	Joback Method
cpg	1183.65	J/mol×K	1130.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321150&Units=SI

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