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

Inchi: InChI=1S/C16H23NO4/c1-4-5-6-10-21-15(18)12-17(2)16(19)13-8-7-9-14(11-13)20-3/h7-9

InchiKey: SLWFAWKKVMTFAT-UHFFFAOYSA-N

Formula: C16H23NO4

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

Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-170.44	kJ/mol	Joback Method
hf	-570.58	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	74.50	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.501		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	762.16	K	Joback Method
tc	962.44	K	Joback Method
tf	485.81	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.07	J/mol×K	762.16	Joback Method
cpg	704.28	J/mol×K	795.54	Joback Method
cpg	718.48	J/mol×K	828.92	Joback Method
cpg	731.71	J/mol×K	862.30	Joback Method
cpg	743.96	J/mol×K	895.68	Joback Method
cpg	755.28	J/mol×K	929.06	Joback Method
cpg	765.67	J/mol×K	962.44	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=U321493&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