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

Inchi: InChI=1S/C14H19NO4/c1-4-8-19-13(16)10-15(2)14(17)11-6-5-7-12(9-11)18-3/h5-7,9H,4

InchiKey: PRMBWZPRHZWKCJ-UHFFFAOYSA-N

Formula: C14H19NO4

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

Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-187.28	kJ/mol	Joback Method
hf	-529.30	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	70.05	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.720		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	716.40	K	Joback Method
tc	920.18	K	Joback Method
tf	463.27	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.34	J/mol×K	716.40	Joback Method
cpg	593.90	J/mol×K	750.36	Joback Method
cpg	607.52	J/mol×K	784.33	Joback Method
cpg	620.22	J/mol×K	818.29	Joback Method
cpg	632.01	J/mol×K	852.25	Joback Method
cpg	642.91	J/mol×K	886.21	Joback Method
cpg	652.92	J/mol×K	920.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321490&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