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

Inchi: InChI=1S/C15H21NO4/c1-11(2)10-20-14(17)9-16(3)15(18)12-6-5-7-13(8-12)19-4/h5-8,11

InchiKey: YTVHSWYUFFFHJE-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: COc1cccc(C(=O)N(C)CC(=O)OCC(C)C)c1

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-181.30	kJ/mol	Joback Method
hf	-555.22	kJ/mol	Joback Method
hfus	33.33	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.966		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2177.00		NIST Webbook
tb	738.84	K	Joback Method
tc	943.66	K	Joback Method
tf	459.54	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.20	J/mol×K	738.84	Joback Method
cpg	649.34	J/mol×K	772.98	Joback Method
cpg	663.48	J/mol×K	807.11	Joback Method
cpg	676.62	J/mol×K	841.25	Joback Method
cpg	688.79	J/mol×K	875.39	Joback Method
cpg	700.00	J/mol×K	909.52	Joback Method
cpg	710.28	J/mol×K	943.66	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=U321491&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