Sarcosine, N-(4-methoxybenzoyl)-, ethyl ester

Inchi: InChI=1S/C13H17NO4/c1-4-18-12(15)9-14(2)13(16)10-5-7-11(17-3)8-6-10/h5-8H,4,9H2,
InchiKey: DLKATLBNWIRJCY-UHFFFAOYSA-N
Formula: C13H17NO4
SMILES: CCOC(=O)CN(C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	-195.70	kJ/mol	Joback Method
hf	-508.66	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.330		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	693.52	K	Joback Method
tc	899.75	K	Joback Method
tf	452.00	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.21	J/mol×K	693.52	Joback Method
cpg	540.37	J/mol×K	727.89	Joback Method
cpg	553.61	J/mol×K	762.26	Joback Method
cpg	565.97	J/mol×K	796.63	Joback Method
cpg	577.44	J/mol×K	831.00	Joback Method
cpg	588.05	J/mol×K	865.37	Joback Method
cpg	597.81	J/mol×K	899.75	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=U321419&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