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

Inchi: InChI=1S/C13H17NO3/c1-4-17-12(15)9-14(3)13(16)11-7-5-10(2)6-8-11/h5-8H,4,9H2,1-3
InchiKey: AQDAELJQZJBFQB-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: CCOC(=O)CN(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-90.70	kJ/mol	Joback Method
hf	-376.44	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.630		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	671.10	K	Joback Method
tc	879.20	K	Joback Method
tf	429.77	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.97	J/mol×K	671.10	Joback Method
cpg	514.45	J/mol×K	705.78	Joback Method
cpg	528.00	J/mol×K	740.47	Joback Method
cpg	540.67	J/mol×K	775.15	Joback Method
cpg	552.47	J/mol×K	809.83	Joback Method
cpg	563.43	J/mol×K	844.52	Joback Method
cpg	573.58	J/mol×K	879.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321212&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