Sarcosine, N-(3-methylbenzoyl)-, butyl ester

Inchi: InChI=1S/C15H21NO3/c1-4-5-9-19-14(17)11-16(3)15(18)13-8-6-7-12(2)10-13/h6-8,10H,
InchiKey: KUNPAORYHJFQEL-UHFFFAOYSA-N
Formula: C15H21NO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-73.86	kJ/mol	Joback Method
hf	-417.72	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	69.87	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.410		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	716.86	K	Joback Method
tc	919.80	K	Joback Method
tf	452.31	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.12	J/mol×K	716.86	Joback Method
cpg	621.39	J/mol×K	750.68	Joback Method
cpg	635.70	J/mol×K	784.51	Joback Method
cpg	649.08	J/mol×K	818.33	Joback Method
cpg	661.55	J/mol×K	852.15	Joback Method
cpg	673.14	J/mol×K	885.98	Joback Method
cpg	683.89	J/mol×K	919.80	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=U321155&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