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

Inchi: InChI=1S/C16H23NO3/c1-3-4-12-20-16(19)13-17(2)15(18)11-10-14-8-6-5-7-9-14/h5-9H,
InchiKey: SHBIARCZZWJDSP-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: CCCCOC(=O)CN(C)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-55.81	kJ/mol	Joback Method
hf	-426.89	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.421		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	734.76	K	Joback Method
tc	934.97	K	Joback Method
tf	451.06	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.66	J/mol×K	734.76	Joback Method
cpg	677.37	J/mol×K	768.13	Joback Method
cpg	692.08	J/mol×K	801.50	Joback Method
cpg	705.82	J/mol×K	834.86	Joback Method
cpg	718.62	J/mol×K	868.23	Joback Method
cpg	730.54	J/mol×K	901.60	Joback Method
cpg	741.59	J/mol×K	934.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321413&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