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

Inchi: InChI=1S/C15H21NO3/c1-3-11-19-15(18)12-16(2)14(17)10-9-13-7-5-4-6-8-13/h4-8H,3,9-

InchiKey: PSVJBJCNVZEEDN-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: CCCOC(=O)CN(C)C(=O)CCc1ccccc1

Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-64.23	kJ/mol	Joback Method
hf	-406.25	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.031		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	711.88	K	Joback Method
tc	914.00	K	Joback Method
tf	439.79	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.84	J/mol×K	711.88	Joback Method
cpg	622.25	J/mol×K	745.57	Joback Method
cpg	636.67	J/mol×K	779.25	Joback Method
cpg	650.13	J/mol×K	812.94	Joback Method
cpg	662.69	J/mol×K	846.63	Joback Method
cpg	674.36	J/mol×K	880.32	Joback Method
cpg	685.18	J/mol×K	914.00	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=U321411&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