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

Inchi: InChI=1S/C16H23NO3/c1-13(2)12-20-16(19)11-17(3)15(18)10-9-14-7-5-4-6-8-14/h4-8,13

InchiKey: QDZPYFPJEZVCBA-UHFFFAOYSA-N

Formula: C16H23NO3

SMILES: CC(C)COC(=O)CN(C)C(=O)CCc1ccccc1

Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-58.25	kJ/mol	Joback Method
hf	-432.17	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.277		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	734.32	K	Joback Method
tc	937.54	K	Joback Method
tf	436.06	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.18	J/mol×K	734.32	Joback Method
cpg	678.15	J/mol×K	768.19	Joback Method
cpg	693.07	J/mol×K	802.06	Joback Method
cpg	706.98	J/mol×K	835.93	Joback Method
cpg	719.92	J/mol×K	869.80	Joback Method
cpg	731.93	J/mol×K	903.67	Joback Method
cpg	743.05	J/mol×K	937.54	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=U321412&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