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

Inchi: InChI=1S/C18H27NO3/c1-15(2)8-7-13-22-18(21)14-19(3)17(20)12-11-16-9-5-4-6-10-16/h
InchiKey: VZMGVUQHLBAYMM-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CC(C)CCCOC(=O)CN(C)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-41.41	kJ/mol	Joback Method
hf	-473.45	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.057		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	780.08	K	Joback Method
tc	980.41	K	Joback Method
tf	458.60	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.99	J/mol×K	780.08	Joback Method
cpg	791.42	J/mol×K	813.47	Joback Method
cpg	806.77	J/mol×K	846.86	Joback Method
cpg	821.08	J/mol×K	880.25	Joback Method
cpg	834.40	J/mol×K	913.63	Joback Method
cpg	846.77	J/mol×K	947.02	Joback Method
cpg	858.23	J/mol×K	980.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321415&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

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