Sarcosine, N-(4-methoxybenzoyl)-, hexyl ester

Inchi: InChI=1S/C17H25NO4/c1-4-5-6-7-12-22-16(19)13-18(2)17(20)14-8-10-15(21-3)11-9-14/h
InchiKey: AKVJNLBWAWJMST-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-162.02	kJ/mol	Joback Method
hf	-591.22	kJ/mol	Joback Method
hfus	42.03	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.891		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	785.04	K	Joback Method
tc	984.36	K	Joback Method
tf	497.08	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.50	J/mol×K	785.04	Joback Method
cpg	760.98	J/mol×K	818.26	Joback Method
cpg	775.41	J/mol×K	851.48	Joback Method
cpg	788.84	J/mol×K	884.70	Joback Method
cpg	801.27	J/mol×K	917.92	Joback Method
cpg	812.73	J/mol×K	951.14	Joback Method
cpg	823.25	J/mol×K	984.36	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=U321424&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