Sarcosine, N-(3-methoxybenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H27NO4/c1-4-5-6-7-8-12-23-17(20)14-19(2)18(21)15-10-9-11-16(13-15)22

InchiKey: NPMNNYYNLWCIEF-UHFFFAOYSA-N

Formula: C18H27NO4

SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-153.60	kJ/mol	Joback Method
hf	-611.86	kJ/mol	Joback Method
hfus	44.62	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.281		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	2523.00		NIST Webbook
tb	807.92	K	Joback Method
tc	1006.87	K	Joback Method
tf	508.35	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.88	J/mol×K	807.92	Joback Method
cpg	818.59	J/mol×K	841.08	Joback Method
cpg	833.23	J/mol×K	874.24	Joback Method
cpg	846.83	J/mol×K	907.40	Joback Method
cpg	859.40	J/mol×K	940.55	Joback Method
cpg	870.98	J/mol×K	973.71	Joback Method
cpg	881.59	J/mol×K	1006.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321496&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