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

Inchi: InChI=1S/C18H27NO3/c1-4-5-6-7-8-12-22-18(21)19-15(3)17(20)16-11-9-10-14(2)13-16/l
InchiKey: HEGKQYXVFPULQI-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCCCCOC(O)=NC(C)C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
hf	-519.67	kJ/mol	Joback Method
hvap	87.44	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.467		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	887.49	K	Joback Method
tc	1095.76	K	Joback Method

Sources

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=U321157&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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

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