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

Inchi: InChI=1S/C19H29NO4/c1-4-5-6-7-8-9-14-24-18(21)15-20(2)19(22)16-10-12-17(23-3)13-
InchiKey: UCHBNPSIEQGBML-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
gf	-145.18	kJ/mol	Joback Method
hf	-632.50	kJ/mol	Joback Method
hfus	47.21	kJ/mol	Joback Method
hvap	81.18	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.671		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	830.80	K	Joback Method
tc	1030.02	K	Joback Method
tf	519.62	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.13	J/mol×K	830.80	Joback Method
cpg	877.06	J/mol×K	864.00	Joback Method
cpg	891.89	J/mol×K	897.21	Joback Method
cpg	905.64	J/mol×K	930.41	Joback Method
cpg	918.33	J/mol×K	963.61	Joback Method
cpg	929.99	J/mol×K	996.82	Joback Method
cpg	940.66	J/mol×K	1030.02	Joback Method

Sources

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=U321426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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