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

Inchi: InChI=1S/C21H33NO3/c1-4-5-6-7-8-9-10-11-15-25-20(23)17-22(3)21(24)19-14-12-13-18
InchiKey: AUDAXUIXZUCITC-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-23.34	kJ/mol	Joback Method
hf	-541.56	kJ/mol	Joback Method
hfus	51.20	kJ/mol	Joback Method
hvap	83.22	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.751		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	854.14	K	Joback Method
tc	1053.99	K	Joback Method
tf	519.93	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.02	J/mol×K	854.14	Joback Method
cpg	966.86	J/mol×K	887.45	Joback Method
cpg	982.58	J/mol×K	920.76	Joback Method
cpg	997.22	J/mol×K	954.06	Joback Method
cpg	1010.84	J/mol×K	987.37	Joback Method
cpg	1023.47	J/mol×K	1020.68	Joback Method
cpg	1035.16	J/mol×K	1053.99	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=U321160&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