Sarcosine, N-(4-methylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C22H35NO3/c1-4-5-6-7-8-9-10-11-12-17-26-21(24)18-23(3)22(25)20-15-13-19
InchiKey: ZSWYINPJXSLSBI-UHFFFAOYSA-N
Formula: C22H35NO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
gf	-14.92	kJ/mol	Joback Method
hf	-562.20	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	85.45	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.141		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2850.00		NIST Webbook
tb	877.02	K	Joback Method
tc	1078.66	K	Joback Method
tf	531.20	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.30	J/mol×K	877.02	Joback Method
cpg	1027.39	J/mol×K	910.63	Joback Method
cpg	1043.32	J/mol×K	944.23	Joback Method
cpg	1058.14	J/mol×K	977.84	Joback Method
cpg	1071.90	J/mol×K	1011.45	Joback Method
cpg	1084.66	J/mol×K	1045.06	Joback Method
cpg	1096.45	J/mol×K	1078.66	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=U321223&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