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

Inchi: InChI=1S/C21H32FNO3/c1-3-4-5-6-7-8-9-10-11-16-26-20(24)17-23(2)21(25)18-12-14-19
InchiKey: DAMWILXBJNAKGD-UHFFFAOYSA-N
Formula: C21H32FNO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 365.48

Physical Properties

Property code	Value	Unit	Source
gf	-218.15	kJ/mol	Joback Method
hf	-737.67	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.972		Crippen Method
mcvol	303.750	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	853.41	K	Joback Method
tc	1050.11	K	Joback Method
tf	520.52	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.32	J/mol×K	853.41	Joback Method
cpg	973.79	J/mol×K	886.19	Joback Method
cpg	989.18	J/mol×K	918.98	Joback Method
cpg	1003.52	J/mol×K	951.76	Joback Method
cpg	1016.86	J/mol×K	984.54	Joback Method
cpg	1029.24	J/mol×K	1017.33	Joback Method
cpg	1040.71	J/mol×K	1050.11	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=U321314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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