Sarcosine, N-(3-fluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H28FNO3/c1-3-4-5-6-7-8-9-13-24-18(22)15-21(2)19(23)16-11-10-12-17(20
InchiKey: CQCULGSDCAAMHH-UHFFFAOYSA-N
Formula: C19H28FNO3
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 337.43

Physical Properties

Property code	Value	Unit	Source
gf	-234.99	kJ/mol	Joback Method
hf	-696.39	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.191		Crippen Method
mcvol	275.570	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2465.00		NIST Webbook
tb	807.65	K	Joback Method
tc	1001.55	K	Joback Method
tf	497.98	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.22	J/mol×K	807.65	Joback Method
cpg	855.12	J/mol×K	839.97	Joback Method
cpg	870.01	J/mol×K	872.28	Joback Method
cpg	883.92	J/mol×K	904.60	Joback Method
cpg	896.89	J/mol×K	936.91	Joback Method
cpg	908.95	J/mol×K	969.23	Joback Method
cpg	920.15	J/mol×K	1001.55	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=U321391&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