Sarcosine, N-(2,6-difluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H27F2NO3/c1-3-4-5-6-7-8-9-13-25-17(23)14-22(2)19(24)18-15(20)11-10-1

InchiKey: WLVAVMFHHVHICE-UHFFFAOYSA-N

Formula: C19H27F2NO3

SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 355.42

Physical Properties

Property code	Value	Unit	Source
gf	-439.43	kJ/mol	Joback Method
hf	-903.97	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.331		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	811.90	K	Joback Method
tc	1002.82	K	Joback Method
tf	511.09	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.08	J/mol×K	811.90	Joback Method
cpg	861.51	J/mol×K	843.72	Joback Method
cpg	875.95	J/mol×K	875.54	Joback Method
cpg	889.45	J/mol×K	907.36	Joback Method
cpg	902.03	J/mol×K	939.18	Joback Method
cpg	913.73	J/mol×K	971.00	Joback Method
cpg	924.59	J/mol×K	1002.82	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=U321299&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