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

Inchi: InChI=1S/C21H31F2NO3/c1-3-4-5-6-7-8-9-10-11-15-27-19(25)16-24(2)21(26)20-17(22)1
InchiKey: ZHIGEAAJDWTZNF-UHFFFAOYSA-N
Formula: C21H31F2NO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 383.47

Physical Properties

Property code	Value	Unit	Source
gf	-422.59	kJ/mol	Joback Method
hf	-945.25	kJ/mol	Joback Method
hfus	56.98	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.111		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	2730.00		NIST Webbook
tb	857.66	K	Joback Method
tc	1052.86	K	Joback Method
tf	533.63	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.07	J/mol×K	857.66	Joback Method
cpg	980.17	J/mol×K	890.19	Joback Method
cpg	995.20	J/mol×K	922.73	Joback Method
cpg	1009.20	J/mol×K	955.26	Joback Method
cpg	1022.21	J/mol×K	987.80	Joback Method
cpg	1034.27	J/mol×K	1020.33	Joback Method
cpg	1045.41	J/mol×K	1052.86	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=U321301&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