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

Inchi: InChI=1S/C13H15F2NO3/c1-3-7-19-11(17)8-16(2)13(18)12-9(14)5-4-6-10(12)15/h4-6H,3

InchiKey: KWPIFXGJDORBCR-UHFFFAOYSA-N

Formula: C13H15F2NO3

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

Mol. weight [g/mol]: 271.26

Physical Properties

Property code	Value	Unit	Source
gf	-489.95	kJ/mol	Joback Method
hf	-780.13	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.990		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1902.00		NIST Webbook
tb	674.62	K	Joback Method
tc	867.65	K	Joback Method
tf	443.47	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.11	J/mol×K	674.62	Joback Method
cpg	528.21	J/mol×K	706.79	Joback Method
cpg	540.54	J/mol×K	738.96	Joback Method
cpg	552.11	J/mol×K	771.14	Joback Method
cpg	562.93	J/mol×K	803.31	Joback Method
cpg	573.03	J/mol×K	835.48	Joback Method
cpg	582.43	J/mol×K	867.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U321293&Units=SI

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