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

Inchi: InChI=1S/C12H13F2NO3/c1-3-18-10(16)7-15(2)12(17)11-8(13)5-4-6-9(11)14/h4-6H,3,7H
InchiKey: ZDPVKSYNOMDJIL-UHFFFAOYSA-N
Formula: C12H13F2NO3
SMILES: CCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 257.23

Physical Properties

Property code	Value	Unit	Source
gf	-498.37	kJ/mol	Joback Method
hf	-759.49	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	62.22	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.600		Crippen Method
mcvol	178.710	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	651.74	K	Joback Method
tc	846.77	K	Joback Method
tf	432.20	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.11	J/mol×K	651.74	Joback Method
cpg	476.68	J/mol×K	684.25	Joback Method
cpg	488.50	J/mol×K	716.75	Joback Method
cpg	499.59	J/mol×K	749.26	Joback Method
cpg	509.97	J/mol×K	781.76	Joback Method
cpg	519.65	J/mol×K	814.27	Joback Method
cpg	528.66	J/mol×K	846.77	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=U321292&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