l-Methionine, N-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H15F2NO3S/c1-19-13(18)10(6-7-20-2)16-12(17)11-8(14)4-3-5-9(11)15/h3-

InchiKey: MGRUJXGGOSXHMQ-UHFFFAOYSA-N

Formula: C13H15F2NO3S

SMILES: COC(=O)C(CCSC)NC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 303.32

Physical Properties

Property code	Value	Unit	Source
gf	-480.66	kJ/mol	Joback Method
hf	-757.60	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	1.989		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	780.69	K	Joback Method
tc	993.55	K	Joback Method
tf	483.06	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.17	J/mol×K	780.69	Joback Method
cpg	593.14	J/mol×K	816.17	Joback Method
cpg	604.15	J/mol×K	851.64	Joback Method
cpg	614.21	J/mol×K	887.12	Joback Method
cpg	623.35	J/mol×K	922.60	Joback Method
cpg	631.57	J/mol×K	958.07	Joback Method
cpg	638.87	J/mol×K	993.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299663&Units=SI
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

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