Glycine, N-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C10H9F2NO3/c1-16-8(14)5-13-10(15)9-6(11)3-2-4-7(9)12/h2-4H,5H2,1H3,(H,1
InchiKey: VPICUYOQVIUOAG-UHFFFAOYSA-N
Formula: C10H9F2NO3
SMILES: COC(=O)CNC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 229.18

Physical Properties

Property code	Value	Unit	Source
gf	-536.60	kJ/mol	Joback Method
hf	-732.27	kJ/mol	Joback Method
hfus	30.56	kJ/mol	Joback Method
hvap	62.16	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.868		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1627.00		NIST Webbook
tb	643.71	K	Joback Method
tc	846.54	K	Joback Method
tf	429.85	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.25	J/mol×K	643.71	Joback Method
cpg	387.93	J/mol×K	677.52	Joback Method
cpg	397.96	J/mol×K	711.32	Joback Method
cpg	407.35	J/mol×K	745.13	Joback Method
cpg	416.10	J/mol×K	778.93	Joback Method
cpg	424.23	J/mol×K	812.74	Joback Method
cpg	431.73	J/mol×K	846.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299661&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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