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

Inchi: InChI=1S/C14H17F2NO3/c1-3-4-8-20-12(18)9-17(2)14(19)13-10(15)6-5-7-11(13)16/h5-7
InchiKey: KKKLIMVPEHCITK-UHFFFAOYSA-N
Formula: C14H17F2NO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 285.29

Physical Properties

Property code	Value	Unit	Source
gf	-481.53	kJ/mol	Joback Method
hf	-800.77	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.380		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2003.00		NIST Webbook
tb	697.50	K	Joback Method
tc	888.92	K	Joback Method
tf	454.74	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.44	J/mol×K	697.50	Joback Method
cpg	581.02	J/mol×K	729.40	Joback Method
cpg	593.79	J/mol×K	761.31	Joback Method
cpg	605.77	J/mol×K	793.21	Joback Method
cpg	616.98	J/mol×K	825.12	Joback Method
cpg	627.45	J/mol×K	857.02	Joback Method
cpg	637.18	J/mol×K	888.92	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=U321294&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