Sarcosine, N-(2-fluorobenzoyl)-, ethyl ester

Inchi: InChI=1S/C12H14FNO3/c1-3-17-11(15)8-14(2)12(16)9-6-4-5-7-10(9)13/h4-7H,3,8H2,1-2
InchiKey: PZFIUMMVZAWMOH-UHFFFAOYSA-N
Formula: C12H14FNO3
SMILES: CCOC(=O)CN(C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 239.24

Physical Properties

Property code	Value	Unit	Source
gf	-293.93	kJ/mol	Joback Method
hf	-551.91	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.461		Crippen Method
mcvol	176.940	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1750.00		NIST Webbook
tb	647.49	K	Joback Method
tc	849.83	K	Joback Method
tf	419.09	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.92	J/mol×K	647.49	Joback Method
cpg	470.24	J/mol×K	681.21	Joback Method
cpg	482.74	J/mol×K	714.94	Joback Method
cpg	494.42	J/mol×K	748.66	Joback Method
cpg	505.33	J/mol×K	782.38	Joback Method
cpg	515.48	J/mol×K	816.10	Joback Method
cpg	524.89	J/mol×K	849.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321239&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