Sarcosine, N-(3-fluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C13H16FNO3/c1-3-7-18-12(16)9-15(2)13(17)10-5-4-6-11(14)8-10/h4-6,8H,3,7
InchiKey: RYPCDFHQFJBZFS-UHFFFAOYSA-N
Formula: C13H16FNO3
SMILES: CCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 253.27

Physical Properties

Property code	Value	Unit	Source
gf	-285.51	kJ/mol	Joback Method
hf	-572.55	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.851		Crippen Method
mcvol	191.030	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1853.00		NIST Webbook
tb	670.37	K	Joback Method
tc	870.15	K	Joback Method
tf	430.36	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.96	J/mol×K	670.37	Joback Method
cpg	521.80	J/mol×K	703.67	Joback Method
cpg	534.78	J/mol×K	736.96	Joback Method
cpg	546.93	J/mol×K	770.26	Joback Method
cpg	558.27	J/mol×K	803.56	Joback Method
cpg	568.82	J/mol×K	836.85	Joback Method
cpg	578.62	J/mol×K	870.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321385&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