Sarcosine, N-(4-trifluoromethylbenzoyl)-, butyl ester

Inchi: InChI=1S/C15H18F3NO3/c1-3-4-9-22-13(20)10-19(2)14(21)11-5-7-12(8-6-11)15(16,17)1

InchiKey: CDDHFWRUHGHOSZ-UHFFFAOYSA-N

Formula: C15H18F3NO3

SMILES: CCCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 317.30

Physical Properties

Property code	Value	Unit	Source
gf	-655.45	kJ/mol	Joback Method
hf	-1014.80	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	66.12	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.121		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	711.44	K	Joback Method
tc	902.02	K	Joback Method
tf	456.50	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.13	J/mol×K	711.44	Joback Method
cpg	646.03	J/mol×K	743.20	Joback Method
cpg	659.03	J/mol×K	774.97	Joback Method
cpg	671.16	J/mol×K	806.73	Joback Method
cpg	682.48	J/mol×K	838.49	Joback Method
cpg	693.01	J/mol×K	870.26	Joback Method
cpg	702.82	J/mol×K	902.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321505&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