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

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

InchiKey: UIRNOCRCQIEJJH-UHFFFAOYSA-N

Formula: C15H18F3NO3

SMILES: CC(C)COC(=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	-657.89	kJ/mol	Joback Method
hf	-1020.08	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	65.73	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.977		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	711.00	K	Joback Method
tc	904.33	K	Joback Method
tf	441.50	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.66	J/mol×K	711.00	Joback Method
cpg	646.78	J/mol×K	743.22	Joback Method
cpg	659.97	J/mol×K	775.44	Joback Method
cpg	672.26	J/mol×K	807.67	Joback Method
cpg	683.69	J/mol×K	839.89	Joback Method
cpg	694.32	J/mol×K	872.11	Joback Method
cpg	704.19	J/mol×K	904.33	Joback Method

Sources

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=U321504&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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