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

Inchi: InChI=1S/C14H16F3NO3/c1-3-8-21-12(19)9-18(2)13(20)10-4-6-11(7-5-10)14(15,16)17/h

InchiKey: YVHRYRDGDCAZNV-UHFFFAOYSA-N

Formula: C14H16F3NO3

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

Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-663.87	kJ/mol	Joback Method
hf	-994.16	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.731		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	688.56	K	Joback Method
tc	880.48	K	Joback Method
tf	445.23	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.93	J/mol×K	688.56	Joback Method
cpg	592.46	J/mol×K	720.55	Joback Method
cpg	605.10	J/mol×K	752.53	Joback Method
cpg	616.88	J/mol×K	784.52	Joback Method
cpg	627.86	J/mol×K	816.51	Joback Method
cpg	638.07	J/mol×K	848.50	Joback Method
cpg	647.56	J/mol×K	880.48	Joback Method

Sources

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=U321503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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