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

Inchi: InChI=1S/C21H30F3NO3/c1-3-4-5-6-7-8-9-10-15-28-19(26)16-25(2)20(27)17-11-13-18(1

InchiKey: VAZPFDHCNOEFKD-UHFFFAOYSA-N

Formula: C21H30F3NO3

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

Mol. weight [g/mol]: 401.46

Physical Properties

Property code	Value	Unit	Source
gf	-604.93	kJ/mol	Joback Method
hf	-1138.64	kJ/mol	Joback Method
hfus	53.03	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.461		Crippen Method
mcvol	307.290	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	848.72	K	Joback Method
tc	1042.82	K	Joback Method
tf	524.12	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.80	J/mol×K	848.72	Joback Method
cpg	988.64	J/mol×K	881.07	Joback Method
cpg	1003.44	J/mol×K	913.42	Joback Method
cpg	1017.27	J/mol×K	945.77	Joback Method
cpg	1030.18	J/mol×K	978.12	Joback Method
cpg	1042.23	J/mol×K	1010.47	Joback Method
cpg	1053.48	J/mol×K	1042.82	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=U321511&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