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

Inchi: InChI=1S/C20H28F3NO3/c1-3-4-5-6-7-8-9-14-27-18(25)15-24(2)19(26)16-10-12-17(13-1

InchiKey: DQROQIASZXELOL-UHFFFAOYSA-N

Formula: C20H28F3NO3

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

Mol. weight [g/mol]: 387.44

Physical Properties

Property code	Value	Unit	Source
gf	-613.35	kJ/mol	Joback Method
hf	-1118.00	kJ/mol	Joback Method
hfus	50.44	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.071		Crippen Method
mcvol	293.200	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2394.00		NIST Webbook
tb	825.84	K	Joback Method
tc	1017.72	K	Joback Method
tf	512.85	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.80	J/mol×K	825.84	Joback Method
cpg	929.30	J/mol×K	857.82	Joback Method
cpg	943.80	J/mol×K	889.80	Joback Method
cpg	957.35	J/mol×K	921.78	Joback Method
cpg	970.00	J/mol×K	953.76	Joback Method
cpg	981.82	J/mol×K	985.74	Joback Method
cpg	992.85	J/mol×K	1017.72	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=U321510&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