Sarcosine, N-(2,3,4-trifluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H26F3NO3/c1-3-4-5-6-7-8-9-12-26-16(24)13-23(2)19(25)14-10-11-15(20)1

InchiKey: SQUCNAVDKXCBDM-UHFFFAOYSA-N

Formula: C19H26F3NO3

SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 373.41

Physical Properties

Property code	Value	Unit	Source
gf	-643.87	kJ/mol	Joback Method
hf	-1111.55	kJ/mol	Joback Method
hfus	54.49	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.470		Crippen Method
mcvol	279.110	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tb	816.15	K	Joback Method
tc	1004.82	K	Joback Method
tf	524.20	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.90	J/mol×K	816.15	Joback Method
cpg	867.90	J/mol×K	847.59	Joback Method
cpg	881.96	J/mol×K	879.04	Joback Method
cpg	895.09	J/mol×K	910.48	Joback Method
cpg	907.34	J/mol×K	941.93	Joback Method
cpg	918.71	J/mol×K	973.37	Joback Method
cpg	929.25	J/mol×K	1004.82	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=U321481&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

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