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

Inchi: InChI=1S/C26H40F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-33-23(31)20-30(2)2

InchiKey: AJQWTFMBLRUJQG-UHFFFAOYSA-N

Formula: C26H40F3NO3

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

Mol. weight [g/mol]: 471.60

Physical Properties

Property code	Value	Unit	Source
gf	-584.93	kJ/mol	Joback Method
hf	-1256.03	kJ/mol	Joback Method
hfus	72.62	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.200		Crippen Method
mcvol	377.740	ml/mol	McGowan Method
pc	837.24	kPa	Joback Method
tb	976.31	K	Joback Method
tc	1201.43	K	Joback Method
tf	603.09	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.16	J/mol×K	976.31	Joback Method
cpg	1295.35	J/mol×K	1013.83	Joback Method
cpg	1312.04	J/mol×K	1051.35	Joback Method
cpg	1327.30	J/mol×K	1088.87	Joback Method
cpg	1341.20	J/mol×K	1126.39	Joback Method
cpg	1353.82	J/mol×K	1163.91	Joback Method
cpg	1365.23	J/mol×K	1201.43	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=U321487&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume