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

Inchi: InChI=1S/C26H40F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-33-24(31)21-30(2)25(3

InchiKey: KSWHNZZAELRZSV-UHFFFAOYSA-N

Formula: C26H40F3NO3

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

Mol. weight [g/mol]: 471.60

Physical Properties

Property code	Value	Unit	Source
gf	-562.83	kJ/mol	Joback Method
hf	-1241.84	kJ/mol	Joback Method
hfus	65.98	kJ/mol	Joback Method
hvap	90.61	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.412		Crippen Method
mcvol	377.740	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	3105.00		NIST Webbook
tb	963.12	K	Joback Method
tc	1181.48	K	Joback Method
tf	580.47	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1278.09	J/mol×K	963.12	Joback Method
cpg	1296.14	J/mol×K	999.51	Joback Method
cpg	1312.91	J/mol×K	1035.91	Joback Method
cpg	1328.50	J/mol×K	1072.30	Joback Method
cpg	1343.01	J/mol×K	1108.69	Joback Method
cpg	1356.54	J/mol×K	1145.09	Joback Method
cpg	1369.19	J/mol×K	1181.48	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=U321515&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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