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

Inchi: InChI=1S/C27H42F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-34-25(32)22-31(2)2

InchiKey: NCNYCOAUIVWPDS-UHFFFAOYSA-N

Formula: C27H42F3NO3

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

Mol. weight [g/mol]: 485.62

Physical Properties

Property code	Value	Unit	Source
gf	-554.41	kJ/mol	Joback Method
hf	-1262.48	kJ/mol	Joback Method
hfus	68.57	kJ/mol	Joback Method
hvap	92.83	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.802		Crippen Method
mcvol	391.830	ml/mol	McGowan Method
pc	814.93	kPa	Joback Method
rinpol	3299.00		NIST Webbook
rinpol	3299.00		NIST Webbook
tb	986.00	K	Joback Method
tc	1212.34	K	Joback Method
tf	591.74	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.88	J/mol×K	986.00	Joback Method
cpg	1359.54	J/mol×K	1023.72	Joback Method
cpg	1376.84	J/mol×K	1061.45	Joback Method
cpg	1392.90	J/mol×K	1099.17	Joback Method
cpg	1407.84	J/mol×K	1136.89	Joback Method
cpg	1421.78	J/mol×K	1174.62	Joback Method
cpg	1434.83	J/mol×K	1212.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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