

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

Inchi:	InChI=1S/C28H44F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-35-26(33)23-32
InchiKey:	WGISACAPDJQNGU-UHFFFAOYSA-N
Formula:	C28H44F3NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	499.65

Physical Properties

Property code	Value	Unit	Source
gf	-545.99	kJ/mol	Joback Method
hf	-1283.12	kJ/mol	Joback Method
hfus	71.16	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.192		Crippen Method
mvol	405.920	ml/mol	McGowan Method
pc	772.03	kPa	Joback Method
tb	1008.88	K	Joback Method
tc	1244.45	K	Joback Method
tf	603.01	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.15	J/molxK	1008.88	Joback Method
cpg	1423.49	J/molxK	1048.14	Joback Method
cpg	1441.39	J/molxK	1087.40	Joback Method
cpg	1457.98	J/molxK	1126.66	Joback Method
cpg	1473.41	J/molxK	1165.92	Joback Method
cpg	1487.81	J/molxK	1205.18	Joback Method
cpg	1501.32	J/molxK	1244.45	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=U321517&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

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