

Sarcosine, n-(4-trifluoromethylbenzoyl)-, propyl ester

Inchi:	InChI=1S/C14H16F3NO3/c1-3-8-21-12(19)9-18(2)13(20)10-4-6-11(7-5-10)14(15,16)17/h
InchiKey:	YVHRYRDGDCAZNV-UHFFFAOYSA-N
Formula:	C14H16F3NO3
SMILES:	CCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	303.28

Physical Properties

Property code	Value	Unit	Source
hfus	34.90	kJ/mol	Joback Method
logp	2.731		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tf	341.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.93	J/mol×K	688.56	Joback Method
cpg	592.46	J/mol×K	720.55	Joback Method
cpg	605.10	J/mol×K	752.53	Joback Method
cpg	616.88	J/mol×K	784.52	Joback Method
cpg	627.86	J/mol×K	816.51	Joback Method
cpg	638.07	J/mol×K	848.50	Joback Method
cpg	647.56	J/mol×K	880.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U321503&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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