

Sarcosine, N-(2-trifluoromethylbenzoyl)-, isoheptyl ester

Inchi:	InChI=1S/C17H22F3NO3/c1-12(2)7-6-10-24-15(22)11-21(3)16(23)13-8-4-5-9-14(13)17(1)
InchiKey:	UNHCWNGVAXYQRG-UHFFFAOYSA-N
Formula:	C17H22F3NO3
SMILES:	CC(C)CCCOC(=O)CN(C)C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	345.36

Physical Properties

Property code	Value	Unit	Source
gf	-641.05	kJ/mol	Joback Method
hf	-1061.36	kJ/mol	Joback Method
hfus	39.15	kJ/mol	Joback Method
hvap	70.18	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.757		Crippen Method
mvol	250.930	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	2088.00		NIST Webbook
tb	756.76	K	Joback Method
tc	948.31	K	Joback Method
tf	464.04	K	Joback Method
vc	0.965	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.41	J/molxK	756.76	Joback Method
cpg	757.15	J/molxK	788.68	Joback Method
cpg	770.93	J/molxK	820.61	Joback Method
cpg	783.79	J/molxK	852.53	Joback Method
cpg	795.77	J/molxK	884.46	Joback Method
cpg	806.93	J/molxK	916.38	Joback Method
cpg	817.31	J/molxK	948.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/12-453-5/Sarcosine-N-2-trifluoromethylbenzoyl-isoheptyl-ester.pdf>

Generated by Cheméo on 2026-06-16 18:57:13.42483649 +0000 UTC m=+5401582.482918711.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.