

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

Inchi:	InChI=1S/C17H22F3NO3/c1-12(2)5-4-10-24-15(22)11-21(3)16(23)13-6-8-14(9-7-13)17(1)
InchiKey:	NWJAVIONMBHMBD-UHFFFAOYSA-N
Formula:	C17H22F3NO3
SMILES:	CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1
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
mcvol	250.930	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpola	2053.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321507&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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