Sarcosine, N-pentafluorobenzoyl-, ethyl ester

Inchi: InChI=1S/C12H10F5NO3/c1-3-21-5(19)4-18(2)12(20)6-7(13)9(15)11(17)10(16)8(6)14/h3
InchiKey: CIUFHJXMOVARRA-UHFFFAOYSA-N
Formula: C12H10F5NO3
SMILES: CCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 311.21

Physical Properties

Property code	Value	Unit	Source
hf	-1253.02	kJ/mol	Cheméo Relay (1.0)
hfus	41.74	kJ/mol	Joback Method
hvap	79.17	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-4.37		Cheméo Relay (1.0)
logp	2.017		Crippen Method
mcvol	184.020	ml/mol	McGowan Method
rinpol	1594.00		NIST Webbook
rinpol	1594.00		NIST Webbook
tb	541.67	K	Cheméo Relay (1.0)
tf	329.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.30	J/mol×K	664.49	Joback Method
cpg	495.99	J/mol×K	694.03	Joback Method
cpg	506.12	J/mol×K	723.58	Joback Method
cpg	515.69	J/mol×K	753.12	Joback Method
cpg	524.71	J/mol×K	782.66	Joback Method
cpg	533.20	J/mol×K	812.21	Joback Method
cpg	541.13	J/mol×K	841.75	Joback Method

Sources

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=U321542&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/119-830-8/Sarcosine-N-pentafluorobenzoyl-ethyl-ester.pdf
Generated by Cheméo on 2026-07-22 05:08:58.527911021 +0000 UTC m=+208034.369796402.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.