Sarcosine, n-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C21H36F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-30-18(28)17-27(2)19(2

InchiKey: XRSLUJIZFJOUJH-UHFFFAOYSA-N

Formula: C21H36F5NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 445.51

Physical Properties

Property code	Value	Unit	Source
gf	-1094.49	kJ/mol	Joback Method
hf	-1764.67	kJ/mol	Joback Method
hfus	58.12	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.277		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	812.37	K	Joback Method
tc	994.64	K	Joback Method
tf	488.78	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.37	J/mol×K	812.37	Joback Method
cpg	1098.23	J/mol×K	842.75	Joback Method
cpg	1115.07	J/mol×K	873.13	Joback Method
cpg	1130.93	J/mol×K	903.51	Joback Method
cpg	1145.88	J/mol×K	933.89	Joback Method
cpg	1159.99	J/mol×K	964.26	Joback Method
cpg	1173.32	J/mol×K	994.64	Joback Method

Sources

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=U320943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume