Sarcosine, n-pentafluoropropionyl-, dodecyl ester

Inchi: InChI=1S/C18H30F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-27-15(25)14-24(2)16(26)17(19,2

InchiKey: WWXGTSBKIFCNNS-UHFFFAOYSA-N

Formula: C18H30F5NO3

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

Mol. weight [g/mol]: 403.43

Physical Properties

Property code	Value	Unit	Source
gf	-1119.75	kJ/mol	Joback Method
hf	-1702.75	kJ/mol	Joback Method
hfus	50.35	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.106		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook
tb	743.73	K	Joback Method
tc	913.21	K	Joback Method
tf	454.97	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.21	J/mol×K	743.73	Joback Method
cpg	918.45	J/mol×K	771.98	Joback Method
cpg	933.80	J/mol×K	800.22	Joback Method
cpg	948.30	J/mol×K	828.47	Joback Method
cpg	962.00	J/mol×K	856.72	Joback Method
cpg	974.94	J/mol×K	884.96	Joback Method
cpg	987.18	J/mol×K	913.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume