Sarcosine, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C18H28F7NO3/c1-3-4-5-6-7-8-9-10-11-12-29-14(27)13-26(2)15(28)16(19,20)1

InchiKey: XNTUYWLAGNHYTI-UHFFFAOYSA-N

Formula: C18H28F7NO3

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

Mol. weight [g/mol]: 439.41

Physical Properties

Property code	Value	Unit	Source
gf	-1506.53	kJ/mol	Joback Method
hf	-2103.72	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.352		Crippen Method
mcvol	295.860	ml/mol	McGowan Method
pc	1042.60	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	739.04	K	Joback Method
tc	906.47	K	Joback Method
tf	458.57	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.34	J/mol×K	739.04	Joback Method
cpg	935.05	J/mol×K	766.95	Joback Method
cpg	949.87	J/mol×K	794.85	Joback Method
cpg	963.84	J/mol×K	822.76	Joback Method
cpg	977.02	J/mol×K	850.66	Joback Method
cpg	989.47	J/mol×K	878.57	Joback Method
cpg	1001.23	J/mol×K	906.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321263&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