Sarcosine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C21H34F7NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-32-17(30)16-29(2)18(31)1

InchiKey: BBWZOJDUVGYTDC-UHFFFAOYSA-N

Formula: C21H34F7NO3

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

Mol. weight [g/mol]: 481.49

Physical Properties

Property code	Value	Unit	Source
gf	-1481.27	kJ/mol	Joback Method
hf	-2165.64	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	70.68	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.522		Crippen Method
mcvol	338.130	ml/mol	McGowan Method
pc	872.74	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	807.68	K	Joback Method
tc	989.21	K	Joback Method
tf	492.38	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.20	J/mol×K	807.68	Joback Method
cpg	1113.61	J/mol×K	837.94	Joback Method
cpg	1129.98	J/mol×K	868.19	Joback Method
cpg	1145.40	J/mol×K	898.45	Joback Method
cpg	1159.95	J/mol×K	928.70	Joback Method
cpg	1173.70	J/mol×K	958.96	Joback Method
cpg	1186.72	J/mol×K	989.21	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=U321265&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