Sarcosine, n-heptafluorobutyryl-, dodecyl ester

Inchi: InChI=1S/C19H30F7NO3/c1-3-4-5-6-7-8-9-10-11-12-13-30-15(28)14-27(2)16(29)17(20,2

InchiKey: KETXVSMXMNGJSG-UHFFFAOYSA-N

Formula: C19H30F7NO3

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

Mol. weight [g/mol]: 453.44

Physical Properties

Property code	Value	Unit	Source
gf	-1498.11	kJ/mol	Joback Method
hf	-2124.36	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.742		Crippen Method
mcvol	309.950	ml/mol	McGowan Method
pc	980.85	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	761.92	K	Joback Method
tc	933.26	K	Joback Method
tf	469.84	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.45	J/mol×K	761.92	Joback Method
cpg	993.68	J/mol×K	790.48	Joback Method
cpg	1008.97	J/mol×K	819.03	Joback Method
cpg	1023.39	J/mol×K	847.59	Joback Method
cpg	1036.99	J/mol×K	876.15	Joback Method
cpg	1049.83	J/mol×K	904.70	Joback Method
cpg	1061.98	J/mol×K	933.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321264&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