l-Methionine, n-heptafluorobutyryl-, decyl ester

Inchi: InChI=1S/C19H30F7NO3S/c1-3-4-5-6-7-8-9-10-12-30-15(28)14(11-13-31-2)27-16(29)17

InchiKey: HKVIGMQBIBQLFG-UHFFFAOYSA-N

Formula: C19H30F7NO3S

SMILES: CCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 485.50

Physical Properties

Property code	Value	Unit	Source
gf	-1488.82	kJ/mol	Joback Method
hf	-2101.83	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.741		Crippen Method
mcvol	326.300	ml/mol	McGowan Method
pc	1005.89	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	867.99	K	Joback Method
tc	1062.67	K	Joback Method
tf	509.43	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.55	J/mol×K	867.99	Joback Method
cpg	1074.40	J/mol×K	900.44	Joback Method
cpg	1088.24	J/mol×K	932.88	Joback Method
cpg	1101.15	J/mol×K	965.33	Joback Method
cpg	1113.21	J/mol×K	997.78	Joback Method
cpg	1124.50	J/mol×K	1030.22	Joback Method
cpg	1135.09	J/mol×K	1062.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320857&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