l-Methionine, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C20H32F7NO3S/c1-3-4-5-6-7-8-9-10-11-13-31-16(29)15(12-14-32-2)28-17(30)

InchiKey: NFPQZRCTTDPSBW-UHFFFAOYSA-N

Formula: C20H32F7NO3S

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

Mol. weight [g/mol]: 499.53

Physical Properties

Property code	Value	Unit	Source
gf	-1480.40	kJ/mol	Joback Method
hf	-2122.47	kJ/mol	Joback Method
hfus	56.97	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.131		Crippen Method
mcvol	340.390	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	890.87	K	Joback Method
tc	1091.26	K	Joback Method
tf	520.70	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.10	J/mol×K	890.87	Joback Method
cpg	1134.48	J/mol×K	924.27	Joback Method
cpg	1148.81	J/mol×K	957.67	Joback Method
cpg	1162.18	J/mol×K	991.06	Joback Method
cpg	1174.66	J/mol×K	1024.46	Joback Method
cpg	1186.36	J/mol×K	1057.86	Joback Method
cpg	1197.34	J/mol×K	1091.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320858&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

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