l-Methionine, n-heptafluorobutyryl-, dodecyl ester

Inchi: InChI=1S/C21H34F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-14-32-17(30)16(13-15-33-2)29-18

InchiKey: NVUPBDDUMSGWCO-UHFFFAOYSA-N

Formula: C21H34F7NO3S

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

Mol. weight [g/mol]: 513.55

Physical Properties

Property code	Value	Unit	Source
gf	-1471.98	kJ/mol	Joback Method
hf	-2143.11	kJ/mol	Joback Method
hfus	59.56	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.521		Crippen Method
mcvol	354.480	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	913.75	K	Joback Method
tc	1120.86	K	Joback Method
tf	531.97	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.31	J/mol×K	913.75	Joback Method
cpg	1195.29	J/mol×K	948.27	Joback Method
cpg	1210.16	J/mol×K	982.79	Joback Method
cpg	1224.02	J/mol×K	1017.31	Joback Method
cpg	1236.97	J/mol×K	1051.82	Joback Method
cpg	1249.12	J/mol×K	1086.34	Joback Method
cpg	1260.55	J/mol×K	1120.86	Joback Method

Sources

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=U320859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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