l-Methionine, n-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C13H18F7NO3S/c1-3-4-6-24-9(22)8(5-7-25-2)21-10(23)11(14,15)12(16,17)13(
InchiKey: RAYWSDPQZFLTFJ-UHFFFAOYSA-N
Formula: C13H18F7NO3S
SMILES: CCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 401.34

Physical Properties

Property code	Value	Unit	Source
gf	-1539.34	kJ/mol	Joback Method
hf	-1977.99	kJ/mol	Joback Method
hfus	38.84	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.401		Crippen Method
mcvol	241.760	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	1631.00		NIST Webbook
tb	730.71	K	Joback Method
tc	908.40	K	Joback Method
tf	441.81	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.16	J/mol×K	730.71	Joback Method
cpg	731.45	J/mol×K	760.32	Joback Method
cpg	742.91	J/mol×K	789.94	Joback Method
cpg	753.58	J/mol×K	819.55	Joback Method
cpg	763.52	J/mol×K	849.17	Joback Method
cpg	772.77	J/mol×K	878.78	Joback Method
cpg	781.38	J/mol×K	908.40	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=U320852&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