l-Methionine, n-heptafluorobutyryl-, isobutyl ester

Inchi: InChI=1S/C13H18F7NO3S/c1-7(2)6-24-9(22)8(4-5-25-3)21-10(23)11(14,15)12(16,17)13(

InchiKey: YOFLPQABMWTVEW-UHFFFAOYSA-N

Formula: C13H18F7NO3S

SMILES: CSCCC(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)OCC(C)C

Mol. weight [g/mol]: 401.34

Physical Properties

Property code	Value	Unit	Source
gf	-1541.78	kJ/mol	Joback Method
hf	-1983.27	kJ/mol	Joback Method
hfus	35.31	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.256		Crippen Method
mcvol	241.760	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	730.27	K	Joback Method
tc	909.75	K	Joback Method
tf	426.81	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.72	J/mol×K	730.27	Joback Method
cpg	732.15	J/mol×K	760.18	Joback Method
cpg	743.72	J/mol×K	790.10	Joback Method
cpg	754.49	J/mol×K	820.01	Joback Method
cpg	764.49	J/mol×K	849.92	Joback Method
cpg	773.79	J/mol×K	879.84	Joback Method
cpg	782.43	J/mol×K	909.75	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=U320851&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