l-Methionine, n-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C12H18F5NO3S/c1-7(2)6-21-9(19)8(4-5-22-3)18-10(20)11(13,14)12(15,16)17/

InchiKey: JSAAYXUMLFCDGI-UHFFFAOYSA-N

Formula: C12H18F5NO3S

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

Mol. weight [g/mol]: 351.33

Physical Properties

Property code	Value	Unit	Source
gf	-1163.42	kJ/mol	Joback Method
hf	-1561.66	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	64.01	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.621		Crippen Method
mcvol	224.130	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1573.00		NIST Webbook
tb	712.08	K	Joback Method
tc	895.68	K	Joback Method
tf	411.94	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.91	J/mol×K	712.08	Joback Method
cpg	660.61	J/mol×K	742.68	Joback Method
cpg	672.47	J/mol×K	773.28	Joback Method
cpg	683.53	J/mol×K	803.88	Joback Method
cpg	693.82	J/mol×K	834.48	Joback Method
cpg	703.39	J/mol×K	865.08	Joback Method
cpg	712.26	J/mol×K	895.68	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=U320911&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