l-Methionine, n-pentafluoropropionyl-, butyl ester

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

InchiKey: UEAIDLXJMDBTQT-UHFFFAOYSA-N

Formula: C12H18F5NO3S

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

Mol. weight [g/mol]: 351.33

Physical Properties

Property code	Value	Unit	Source
gf	-1160.98	kJ/mol	Joback Method
hf	-1556.38	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.765		Crippen Method
mcvol	224.130	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	712.52	K	Joback Method
tc	893.87	K	Joback Method
tf	426.94	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.37	J/mol×K	712.52	Joback Method
cpg	659.89	J/mol×K	742.74	Joback Method
cpg	671.60	J/mol×K	772.97	Joback Method
cpg	682.54	J/mol×K	803.19	Joback Method
cpg	692.74	J/mol×K	833.42	Joback Method
cpg	702.23	J/mol×K	863.64	Joback Method
cpg	711.06	J/mol×K	893.87	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320912&Units=SI

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