l-Methionine, n-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C11H16F5NO3S/c1-3-5-20-8(18)7(4-6-21-2)17-9(19)10(12,13)11(14,15)16/h7H

InchiKey: IZMMKWNAFXBTHN-UHFFFAOYSA-N

Formula: C11H16F5NO3S

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

Mol. weight [g/mol]: 337.31

Physical Properties

Property code	Value	Unit	Source
gf	-1169.40	kJ/mol	Joback Method
hf	-1535.74	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.375		Crippen Method
mcvol	210.040	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	689.64	K	Joback Method
tc	871.35	K	Joback Method
tf	415.67	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.69	J/mol×K	689.64	Joback Method
cpg	606.78	J/mol×K	719.92	Joback Method
cpg	618.09	J/mol×K	750.21	Joback Method
cpg	628.64	J/mol×K	780.49	Joback Method
cpg	638.47	J/mol×K	810.78	Joback Method
cpg	647.62	J/mol×K	841.06	Joback Method
cpg	656.11	J/mol×K	871.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320910&Units=SI
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

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