Asparagine, N-trifluoroacetyl, 1-methylethyl ester

Inchi: InChI=1S/C9H13F3N2O4/c1-4(2)18-7(16)5(3-6(13)15)14-8(17)9(10,11)12/h4-5H,3H2,1-2

InchiKey: UGWVCQFPDLOFQH-UHFFFAOYSA-N

Formula: C9H13F3N2O4

SMILES: CC(C)OC(=O)C(CC(N)=O)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 270.21

Physical Properties

Property code	Value	Unit	Source
gf	-897.49	kJ/mol	Joback Method
hf	-1219.43	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	-0.139		Crippen Method
mcvol	173.520	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1379.00		NIST Webbook
tb	705.75	K	Joback Method
tc	898.90	K	Joback Method
tf	473.32	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.24	J/mol×K	705.75	Joback Method
cpg	505.63	J/mol×K	737.94	Joback Method
cpg	515.31	J/mol×K	770.13	Joback Method
cpg	524.30	J/mol×K	802.33	Joback Method
cpg	532.63	J/mol×K	834.52	Joback Method
cpg	540.31	J/mol×K	866.71	Joback Method
cpg	547.37	J/mol×K	898.90	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=R84388&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