Aspartic acid, n-(trifluoroacetyl)-, 1-ethyl ester

Inchi: InChI=1S/C8H10F3NO5/c1-2-17-6(15)4(3-5(13)14)12-7(16)8(9,10)11/h4H,2-3H2,1H3,(H
InchiKey: JHTXBKMSNPTYOR-UHFFFAOYSA-N
Formula: C8H10F3NO5
SMILES: CCOC(=O)C(CC(=O)O)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 257.16
CAS: 45203-86-9

Physical Properties

Property code	Value	Unit	Source
gf	-1106.74	kJ/mol	Joback Method
hf	-1379.53	kJ/mol	Joback Method
hfus	29.95	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.071		Crippen Method
mcvol	155.320	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	702.96	K	Joback Method
tc	881.72	K	Joback Method
tf	454.61	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.65	J/mol×K	702.96	Joback Method
cpg	443.95	J/mol×K	732.75	Joback Method
cpg	451.72	J/mol×K	762.55	Joback Method
cpg	458.96	J/mol×K	792.34	Joback Method
cpg	465.70	J/mol×K	822.13	Joback Method
cpg	471.95	J/mol×K	851.92	Joback Method
cpg	477.74	J/mol×K	881.72	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=C45203869&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume