Ethyl 3-amino-4,4,4-trifluorocrotonate

Other names: 2-Butenoic acid, 3-amino-4,4,4-trifluoro-, ethyl ester
Inchi: InChI=1S/C6H8F3NO2/c1-2-12-5(11)3-4(10)6(7,8)9/h3H,2,10H2,1H3/b4-3-
InchiKey: NXVKRKUGIINGHD-ARJAWSKDSA-N
Formula: C6H8F3NO2
SMILES: CCOC(=O)C=C(N)C(F)(F)F
Mol. weight [g/mol]: 183.13
CAS: 372-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-677.75	kJ/mol	Joback Method
hf	-867.83	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.954		Crippen Method
mcvol	113.830	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	484.12	K	Joback Method
tc	669.33	K	Joback Method
tf	297.95	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.81	J/mol×K	484.12	Joback Method
cpg	271.42	J/mol×K	514.99	Joback Method
cpg	280.47	J/mol×K	545.86	Joback Method
cpg	288.97	J/mol×K	576.72	Joback Method
cpg	296.95	J/mol×K	607.59	Joback Method
cpg	304.44	J/mol×K	638.46	Joback Method
cpg	311.46	J/mol×K	669.33	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=C372292&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume