

Ethyl 3-aminocrotonate

Other names:	3-Aminocrotonic acid ethyl ester Crotonic acid, 3-amino-, ethyl ester Ethyl 3-amino-2-butenate Ethyl 3-aminocrotonate Ethyl «beta»-aminocrotonate «beta»-Aminocrotonic acid ethyl ester
Inchi:	InChI=1S/C6H11NO2/c1-3-9-6(8)4-5(2)7/h4H,3,7H2,1-2H3
InchiKey:	YPMPTULBFPFSEQ-SNAWJCMRSA-N
Formula:	C6H11NO2
SMILES:	CCOC(=O)C=C(C)N
Mol. weight [g/mol]:	129.16
CAS:	626-34-6

Physical Properties

Property code	Value	Unit	Source
af	0.5305		Cheméo Relay (1.0)
gf	-96.16	kJ/mol	Joback Method
hf	-429.91	kJ/mol	Cheméo Relay (1.0)
hfus	18.17	kJ/mol	Joback Method
hvap	59.65	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.16		Cheméo Relay (1.0)
logp	0.412		Crippen Method
mcvol	108.520	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	485.70	K	NIST Webbook
tc	642.12	K	Cheméo Relay (1.0)
tf	314.76	K	Cheméo Relay (1.0)
vc	0.393	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.39	J/mol×K	489.54	Joback Method

cpg	243.60	J/mol×K	523.39	Joback Method
cpg	253.33	J/mol×K	557.24	Joback Method
cpg	262.57	J/mol×K	591.09	Joback Method
cpg	271.35	J/mol×K	624.94	Joback Method
cpg	279.69	J/mol×K	658.78	Joback Method
cpg	287.58	J/mol×K	692.63	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626346&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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