2-Butenamide, N-(aminocarbonyl)-2-ethyl-, (Z)-

Other names:

Ectylurea
Urea, (2-ethylcrotonoyl)-, (Z)-
(«alpha»-Ethyl-cis-crotonyl)carbamide
(2-Ethyl-cis-crotonyl)urea
Ectylcarbamide
Levanil
Nastyn
Nostyn
cis-(2-Ethylcrotonyl) urea
Actine
Astyn
A18285
Cronil
Crotural
Disteol
Distessol
Ectida
Ectilurea
Ecton
Ectyda
Ectyn
Ektyl
Ektylcarbamid
Euplacid
Levil
MA-110
Neocrosedin
Nestyn
Neuroprocin
Nostal
Nostin
Pacetyn
Sedarex
Tranzer
U 8771
Urea, (2-ethylcrotonoyl)-, cis-
(Z)-N-(Aminocarbonyl)-2-ethyl-2-butenamide
(«alpha»-Ethylcrotonyl)urea, (Z)-
N-[(2Z)-2-Ethyl-2-butenoyl]urea
2-Ethylcrotonylurea, (Z)-

Inchi: InChI=1S/C7H12N2O2/c1-3-5(4-2)6(10)9-7(8)11/h3H,4H2,1-2H3,(H3,8,9,10,11)/b5-3-
InchiKey: QCUPYFTWJOZAOB-HYXAFXHYSA-N
Formula: C7H12N2O2
SMILES: CC=C(CC)C(=O)NC(N)=O
Mol. weight [g/mol]: 156.18
CAS: 95-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-22.27	kJ/mol	Joback Method
hf	-218.28	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	61.78	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	0.538		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	594.04	K	Joback Method
tc	805.10	K	Joback Method
tf	385.39	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.08	J/mol×K	594.04	Joback Method
cpg	321.70	J/mol×K	629.22	Joback Method
cpg	331.68	J/mol×K	664.39	Joback Method
cpg	341.03	J/mol×K	699.57	Joback Method
cpg	349.81	J/mol×K	734.75	Joback Method
cpg	358.03	J/mol×K	769.92	Joback Method
cpg	365.74	J/mol×K	805.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95045&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