1-(2-Ethylcrotonoyl)urea

Other names:	2-Butenamide, N-(aminocarbonyl)-2-ethyl- («alpha»-Ethylcrotonyl)carbamide («alpha»-Ethylcrotonyl)urea (2-Ethylcrotonoyl)urea Crotonyl ureide, «alpha»-ethyl- Urea, («alpha»-ethylcrotonoyl)- Urea, (2-ethylcrotonoyl)- N-(2-Ethyl-2-butenoyl)urea NSC 163913 Urea, 2-ethylcrotonyl- N-(aminocarbonyl)-2-ethyl-2-butenamide
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-HWKANZROSA-N
Formula:	C7H12N2O2
SMILES:	CC=C(CC)C(=O)NC(N)=O
Mol. weight [g/mol]:	156.18
CAS:	5982-97-8

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
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

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=C5982978&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