2-BUTYNEDIAMIDE

Other names:	Acetylenedicarboxylic acid diamide
	Aquamycin
	Cellocidin
	Lenamycin
	2-Butynediamide
	Acetylendicarbonsaeureamid
	Renamycin
Inchi:	InChI=1S/C4H4N2O2/c5-3(7)1-2-4(6)8/h(H2,5,7)(H2,6,8)
InchiKey:	JBTGHKUTYAMZEZ-UHFFFAOYSA-N
Formula:	C4H4N2O2
SMILES:	NC(=O)C#CC(N)=O
Mol. weight [g/mol]:	112.09

Physical Properties

Property code	Value	Unit	Source
hf	-190.89	kJ/mol	Cheméo Relay (1.0)
hfus	22.83	kJ/mol	Joback Method
ie	10.12	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	-2.040		Crippen Method
mcvol	81.720	ml/mol	McGowan Method
tf	468.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.43	J/mol×K	552.72	Joback Method
cpg	174.50	J/mol×K	593.81	Joback Method
cpg	180.17	J/mol×K	634.89	Joback Method
cpg	185.46	J/mol×K	675.98	Joback Method
cpg	190.36	J/mol×K	717.06	Joback Method
cpg	194.90	J/mol×K	758.15	Joback Method
cpg	199.08	J/mol×K	799.24	Joback Method

Sources

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=C543215&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point