

Acetylene dicarboxamide

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:	JBTGCHKUTYAMZEE-UHFFFAOYSA-N
Formula:	C4H4N2O2
SMILES:	NC(=O)C#CC(N)=O
Mol. weight [g/mol]:	112.09
CAS:	543-21-5

Physical Properties

Property code	Value	Unit	Source
gf	60.66	kJ/mol	Joback Method
hf	-11.17	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	0.29		Crippen Method
logp	-2.040		Crippen Method
mvol	81.720	ml/mol	McGowan Method
pc	6921.35	kPa	Joback Method
tb	552.72	K	Joback Method
tc	799.24	K	Joback Method
tf	507.32	K	Joback Method
vc	0.291	m ³ /kmol	Joback Method

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:	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=C543215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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