

Guanidine carbonate

Other names:	Guanidinium carbonate Carbonic acid, compd. with guanidine (1:2) Bisguanidinium carbonate Diguanidinium carbonate
Inchi:	InChI=1S/C3H12N6O3/c4-2(5,6)11-1(10)12-3(7,8)9/h4-9H2
InchiKey:	TUXRBQHZZFVXLV-UHFFFAOYSA-N
Formula:	C3H12N6O3
SMILES:	NC(N)(N)OC(=O)OC(N)(N)N
Mol. weight [g/mol]:	180.17
CAS:	593-85-1

Physical Properties

Property code	Value	Unit	Source
gf	39.84	kJ/mol	Joback Method
hf	-297.03	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	0.19		Crippen Method
logp	-3.886		Crippen Method
mcvol	126.320	ml/mol	McGowan Method
pc	8309.73	kPa	Joback Method
ss	295.35	J/mol×K	NIST Webbook
tb	795.47	K	Joback Method
tc	1055.77	K	Joback Method
tf	722.36	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.13	J/mol×K	795.47	Joback Method
cpg	398.40	J/mol×K	838.85	Joback Method
cpg	404.88	J/mol×K	882.24	Joback Method
cpg	410.61	J/mol×K	925.62	Joback Method

cpg	415.66	J/mol×K	969.00	Joback Method
cpg	420.08	J/mol×K	1012.38	Joback Method
cpg	423.94	J/mol×K	1055.77	Joback Method
cps	258.86	J/mol×K	298.10	NIST Webbook

Sources

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=C593851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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