

Glutarimide

Other names:	2,6-Piperidinedione
Inchi:	InChI=1S/C5H7NO2/c7-4-2-1-3-5(8)6-4/h1-3H2,(H,6,7,8)
InchiKey:	KNCYXPMJDCCGSJ-UHFFFAOYSA-N
Formula:	C5H7NO2
SMILES:	O=C1CCCC(=O)N1
Mol. weight [g/mol]:	113.11
CAS:	1121-89-7

Physical Properties

Property code	Value	Unit	Source
chs	-2480.30 ± 0.50	kJ/mol	NIST Webbook
gf	-134.09	kJ/mol	Joback Method
hf	-393.60 ± 1.80	kJ/mol	NIST Webbook
hfs	-487.70 ± 0.80	kJ/mol	NIST Webbook
hfus	8.08	kJ/mol	Joback Method
hsub	94.10 ± 1.60	kJ/mol	NIST Webbook
hsub	94.10 ± 1.60	kJ/mol	NIST Webbook
hvap	42.71	kJ/mol	Joback Method
ie	9.87	eV	NIST Webbook
log10ws	-0.55		Crippen Method
logp	-0.187		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
rinpol	1153.90		NIST Webbook
rinpol	1153.90		NIST Webbook
tb	522.21	K	Joback Method
tc	779.01	K	Joback Method
tf	399.20	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.56	J/mol×K	522.21	Joback Method

cpg	194.50	J/mol×K	565.01	Joback Method
cpg	206.97	J/mol×K	607.81	Joback Method
cpg	218.89	J/mol×K	650.61	Joback Method
cpg	230.17	J/mol×K	693.41	Joback Method
cpg	240.74	J/mol×K	736.21	Joback Method
cpg	250.51	J/mol×K	779.01	Joback Method
hsubt	93.60 ± 1.60	kJ/mol	328.50	NIST Webbook

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=C1121897&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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