

3,3-TETRAMETHYLENEGLUTARIMIDE

Other names:	3,3-Tetramethyleneglutarimide 8-Azaspiro[4.5]decane-7,9-dione
Inchi:	InChI=1S/C9H13NO2/c11-7-5-9(3-1-2-4-9)6-8(12)10-7/h1-6H2,(H,10,11,12)
InchiKey:	YRTHJMQKDCXPAY-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	O=C1CC2(CCCC2)CC(=O)N1
Mol. weight [g/mol]:	167.21

Physical Properties

Property code	Value	Unit	Source
hf	-431.24	kJ/mol	Cheméo Relay (1.0)
hfus	8.18	kJ/mol	Joback Method
hsub	106.80 ± 2.00	kJ/mol	NIST Webbook
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-1.42		Cheméo Relay (1.0)
logp	0.983		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
tb	576.48	K	Cheméo Relay (1.0)
tf	461.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.46	J/mol×K	624.98	Joback Method
cpg	370.22	J/mol×K	670.62	Joback Method
cpg	387.84	J/mol×K	716.25	Joback Method
cpg	404.46	J/mol×K	761.89	Joback Method
cpg	420.22	J/mol×K	807.52	Joback Method
cpg	435.26	J/mol×K	853.16	Joback Method
cpg	449.72	J/mol×K	898.79	Joback Method
hfust	24.20	kJ/mol	426.60	NIST Webbook

Sources

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=C1075894&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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