

3,3-Tetramethyleneglutaric acid

Other names:	«beta», «beta»-tetramethyleneglutaric acid 1,1-Cyclopentanediacetic acid Tetramethyleneglutaric acid TMG 3,3'-Tetramethylene glutaric acid (1-Carboxymethyl-cyclopentyl)-acetic acid cyclopentane-1,1-diacetic acid
Inchi:	InChI=1S/C9H14O4/c10-7(11)5-9(6-8(12)13)3-1-2-4-9/h1-6H2,(H,10,11)(H,12,13)
InchiKey:	FWPVKDFOUXHOKQ-UHFFFAOYSA-N
Formula:	C9H14O4
SMILES:	O=C(O)CC1(CC(=O)O)CCCC1
Mol. weight [g/mol]:	186.21
CAS:	16713-66-9

Physical Properties

Property code	Value	Unit	Source
gf	-475.52	kJ/mol	Joback Method
hf	-682.99	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hsub	126.90 ± 2.40	kJ/mol	NIST Webbook
hvap	81.58	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.496		Crippen Method
mvol	141.690	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	712.94	K	Joback Method
tc	907.37	K	Joback Method
tf	447.49	K	Joback Method
vc	0.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.63	J/mol×K	874.96	Joback Method

cpg	405.85	J/mol×K	712.94	Joback Method
cpg	415.97	J/mol×K	745.34	Joback Method
cpg	425.72	J/mol×K	777.75	Joback Method
cpg	435.18	J/mol×K	810.15	Joback Method
cpg	444.46	J/mol×K	842.56	Joback Method
cpg	462.78	J/mol×K	907.37	Joback Method
hfust	32.10	kJ/mol	452.90	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=C16713669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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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