3,3-Tetramethyleneglutaric anhydride

Other names:	«beta»,«beta»-Tetramethyleneglutaric anhydride
	1,1-Cyclopentanediacetic anhydride
	8-Oxaspiro[4.5]decane-7,9-dione
	cyclopentane-1,1-diacetic anhydride
	3,3-Tetramethyleneglutaric acid anhydride
Inchi:	InChI=1S/C9H12O3/c10-7-5-9(3-1-2-4-9)6-8(11)12-7/h1-6H2
InchiKey:	GFWLMILMVMCJDI-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	O=C1CC2(CCCC2)CC(=O)O1
Mol. weight [g/mol]:	168.19
CAS:	5662-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-231.08	kJ/mol	Joback Method
hf	-479.95	kJ/mol	Joback Method
hfus	6.57	kJ/mol	Joback Method
hsub	96.40 ± 1.10	kJ/mol	NIST Webbook
hvap	48.30	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.410		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	603.38	K	Joback Method
tc	870.54	K	Joback Method
tf	404.14	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.14	J/mol×K	603.38	Joback Method
cpg	355.15	J/mol×K	647.91	Joback Method
cpg	372.02	J/mol×K	692.43	Joback Method

cpg	387.88	J/mol×K	736.96	Joback Method
cpg	402.88	J/mol×K	781.48	Joback Method
cpg	417.16	J/mol×K	826.01	Joback Method
cpg	430.86	J/mol×K	870.54	Joback Method
hfust	15.30	kJ/mol	338.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5662953&Units=SI
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

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