Ethane, 1,1,1-trinitro-

Other names: 1,1,1-Trinitroethane
Inchi: InChI=1S/C2H3N3O6/c1-2(3(6)7,4(8)9)5(10)11/h1H3
InchiKey: HSYGKEBJFKQOLE-UHFFFAOYSA-N
Formula: C2H3N3O6
SMILES: CC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 165.06
CAS: 595-86-8

Physical Properties

Property code	Value	Unit	Source
gf	75.45	kJ/mol	Joback Method
hf	-125.64	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	-0.510		Crippen Method
mcvol	91.300	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
tb	697.45	K	Joback Method
tc	985.78	K	Joback Method
tf	545.55	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.38	J/mol×K	697.45	Joback Method
cpg	239.75	J/mol×K	745.51	Joback Method
cpg	245.33	J/mol×K	793.56	Joback Method
cpg	250.23	J/mol×K	841.62	Joback Method
cpg	254.53	J/mol×K	889.67	Joback Method
cpg	258.33	J/mol×K	937.73	Joback Method
cpg	261.73	J/mol×K	985.78	Joback Method

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=C595868&Units=SI

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
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