2,2,2-Trinitro-1-phenylethane

Inchi: InChI=1S/C8H7N3O6/c12-9(13)8(10(14)15,11(16)17)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: AJYDBHCFRVMOBB-UHFFFAOYSA-N
Formula: C8H7N3O6
SMILES: O=[N+]([O-])C(Cc1ccccc1)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 241.16
CAS: 38677-56-4

Physical Properties

Property code	Value	Unit	Source
chs	-4130.00 ± 4.00	kJ/mol	NIST Webbook
gf	238.38	kJ/mol	Joback Method
hf	65.70 ± 4.20	kJ/mol	NIST Webbook
hfs	-18.00 ± 4.00	kJ/mol	NIST Webbook
hfus	37.19	kJ/mol	Joback Method
hsub	84.10 ± 0.40	kJ/mol	NIST Webbook
hvap	84.16	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	0.713		Crippen Method
mcvol	152.080	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	861.41	K	Joback Method
tc	1158.38	K	Joback Method
tf	639.59	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.32	J/mol×K	861.41	Joback Method
cpg	440.75	J/mol×K	910.90	Joback Method
cpg	448.25	J/mol×K	960.40	Joback Method
cpg	454.98	J/mol×K	1009.89	Joback Method
cpg	461.13	J/mol×K	1059.39	Joback Method
cpg	466.86	J/mol×K	1108.88	Joback Method

cpg	472.36	J/mol×K	1158.38	Joback Method
hsubt	84.10 ± 0.40	kJ/mol	300.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38677564&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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