Triethylenetetramine

Inchi: InChI=1S/C6H18N4/c7-1-3-9-5-6-10-4-2-8/h9-10H,1-8H2
InchiKey: VILCJCGEZXAXTO-UHFFFAOYSA-N
Formula: C6H18N4
SMILES: NCCNCCNCCN
Mol. weight [g/mol]: 146.23
CAS: 39421-77-7

Physical Properties

Property code	Value	Unit	Source
gf	311.32	kJ/mol	Joback Method
hf	7.35	kJ/mol	Joback Method
hfus	31.89	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Joback Method
log10ws	0.42		Crippen Method
logp	-1.917		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1421.00		NIST Webbook
ripol	2154.00		NIST Webbook
tb	582.08	K	Joback Method
tc	777.74	K	Joback Method
tf	429.22	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.25	J/mol×K	582.08	Joback Method
cpg	370.59	J/mol×K	614.69	Joback Method
cpg	382.31	J/mol×K	647.30	Joback Method
cpg	393.41	J/mol×K	679.91	Joback Method
cpg	403.93	J/mol×K	712.52	Joback Method
cpg	413.88	J/mol×K	745.13	Joback Method
cpg	423.29	J/mol×K	777.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39421777&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume