

N,N,N',N'-TETRAETHYL-1,3-PROPANEDIAMINE

Other names:	N,N,N',N'-Tetraethyl trimethylene diamine
Inchi:	InChI=1S/C11H26N2/c1-5-12(6-2)10-9-11-13(7-3)8-4/h5-11H2,1-4H3
InchiKey:	RCZLVPFECJNLMZ-UHFFFAOYSA-N
Formula:	C11H26N2
SMILES:	CCN(CC)CCCN(CC)CC
Mol. weight [g/mol]:	186.34

Physical Properties

Property code	Value	Unit	Source
af	0.5289		Cheméo Relay (1.0)
gf	263.30	kJ/mol	Joback Method
hf	-171.10	kJ/mol	Cheméo Relay (1.0)
hfus	30.29	kJ/mol	Joback Method
hvap	56.73	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-0.98		Cheméo Relay (1.0)
logp	2.060		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
tb	478.34	K	Cheméo Relay (1.0)
tc	642.24	K	Cheméo Relay (1.0)
tf	185.26	K	Cheméo Relay (1.0)
vc	0.698	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.46	J/mol×K	475.96	Joback Method
cpg	445.82	J/mol×K	502.51	Joback Method
cpg	462.47	J/mol×K	529.07	Joback Method
cpg	478.42	J/mol×K	555.62	Joback Method
cpg	493.71	J/mol×K	582.18	Joback Method
cpg	508.34	J/mol×K	608.73	Joback Method
cpg	522.35	J/mol×K	635.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	11.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60558965&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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