

TETRABUTYLUREA

Other names:	Tetrabutylurea tetra-n-Butyl urea
Inchi:	InChI=1S/C17H36N2O/c1-5-9-13-18(14-10-6-2)17(20)19(15-11-7-3)16-12-8-4/h5-16H2,1
InchiKey:	SNDGLCYBKKJSOT-UHFFFAOYSA-N
Formula:	C17H36N2O
SMILES:	CCCCN(CCCC)C(=O)N(CCCC)CCCC
Mol. weight [g/mol]:	284.49

Physical Properties

Property code	Value	Unit	Source
af	0.8570		Cheméo Relay (1.0)
gf	184.90	kJ/mol	Joback Method
hf	-477.41	kJ/mol	Cheméo Relay (1.0)
hfus	47.43	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-3.41		Cheméo Relay (1.0)
logp	4.911		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
tb	580.80	K	Cheméo Relay (1.0)
tc	766.96	K	Cheméo Relay (1.0)
tf	254.68	K	Cheméo Relay (1.0)
vc	1.040	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.40	J/mol×K	667.11	Joback Method
cpg	802.45	J/mol×K	694.81	Joback Method
cpg	820.62	J/mol×K	722.51	Joback Method
cpg	837.95	J/mol×K	750.21	Joback Method
cpg	854.46	J/mol×K	777.91	Joback Method
cpg	870.20	J/mol×K	805.61	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4559868&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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