

PHOSPHINE, TRIBUTYL-

Other names:	(n-C4H9)3P Tri-n-butylphosphine Tributylfosfin Tributylphosphine Tributylphosphorus Tris(butyl)phosphine
Inchi:	InChI=1S/C12H27P/c1-4-7-10-13(11-8-5-2)12-9-6-3/h4-12H2,1-3H3
InchiKey:	TUQOTMZNTHZOKS-UHFFFAOYSA-N
Formula:	C12H27P
SMILES:	CCCCP(CCCC)CCCC
Mol. weight [g/mol]:	202.32

Physical Properties

Property code	Value	Unit	Source
af	0.5383		Cheméo Relay (1.0)
gf	76.13	kJ/mol	Cheméo Relay (1.0, beta)
hf	-313.65	kJ/mol	Cheméo Relay (1.0)
hvap	55.89	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	NIST Webbook
ie	8.00 ± 0.05	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-5.04		Cheméo Relay (1.0)
logp	4.869		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1886.91	kPa	Cheméo Relay (1.0, beta)
tb	495.23	K	Cheméo Relay (1.0)
tc	660.45	K	Cheméo Relay (1.0)
tf	211.59	K	Cheméo Relay (1.0)
vc	0.741	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	51.70 ± 0.50	kJ/mol	390.50	NIST Webbook

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=C998403&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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