

Boric acid (H3BO3), trimethyl ester

Other names:

B(OCH3)3
Borester O
Methyl borate
Methyl borate, ((MeO)3B)
NSC 777
Trimethoxyborane
Trimethoxyborine
Trimethoxyboron
Trimethyl borate
Trimethylester kyseliny borite
UN 2416

Inchi:

InChI=1S/C3H9BO3/c1-5-4(6-2)7-3/h1-3H3

InchiKey:

WRECIMRULFAWHA-UHFFFAOYSA-N

Formula:

C3H9BO3

SMILES:

COB(OC)OC

Mol. weight [g/mol]:

103.91

CAS:

121-43-7

Physical Properties

Property code	Value	Unit	Source
affp	815.80	kJ/mol	NIST Webbook
basg	783.40	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.80 ± 0.30	eV	NIST Webbook
ie	8.90 ± 0.20	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
logp	-0.090		Crippen Method
rinpol	593.00		NIST Webbook
tb	341.90 ± 0.50	K	NIST Webbook
tb	341.80 ± 0.30	K	NIST Webbook
tb	341.62 ± 0.20	K	NIST Webbook
tb	341.99 ± 0.40	K	NIST Webbook
tf	243.90 ± 0.50	K	NIST Webbook
tf	239.15 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	189.90	J/mol×K	298.15	NIST Webbook
hvapt	34.20	kJ/mol	322.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.08313e+01
Coeff. B	-1.18754e+03
Coeff. C	-1.49511e+02
Temperature range (K), min.	259.15
Temperature range (K), max.	364.65

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121437&Units=SI
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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy

logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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