

Amyl-t-butyl ether

Inchi:	InChI=1S/C9H20O/c1-5-6-7-8-10-9(2,3)4/h5-8H2,1-4H3
InchiKey:	BWRSHLROMAZEBM-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCCOC(C)(C)C
Mol. weight [g/mol]:	144.25
CAS:	10100-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-77.26	kJ/mol	Joback Method
hf	-380.60 ± 6.80	kJ/mol	NIST Webbook
hfus	12.84	kJ/mol	Joback Method
hvap	46.30	kJ/mol	NIST Webbook
hvap	46.89 ± 0.99	kJ/mol	NIST Webbook
hvap	46.90 ± 1.00	kJ/mol	NIST Webbook
hvap	48.30	kJ/mol	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.992		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	424.51	K	Joback Method
tc	598.00	K	Joback Method
tf	215.84	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.63	J/mol×K	598.00	Joback Method
cpg	370.42	J/mol×K	569.09	Joback Method
cpg	357.65	J/mol×K	540.17	Joback Method
cpg	344.30	J/mol×K	511.26	Joback Method
cpg	330.37	J/mol×K	482.34	Joback Method
cpg	315.82	J/mol×K	453.43	Joback Method

cpg	300.66	J/mol×K	424.51	Joback Method
dvisc	0.0071777	Pa×s	215.84	Joback Method
dvisc	0.0002250	Pa×s	424.51	Joback Method
dvisc	0.0003097	Pa×s	389.73	Joback Method
dvisc	0.0004539	Pa×s	354.95	Joback Method
dvisc	0.0007228	Pa×s	320.17	Joback Method
dvisc	0.0012893	Pa×s	285.40	Joback Method
dvisc	0.0027004	Pa×s	250.62	Joback Method
hvapt	43.70	kJ/mol	342.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10100955&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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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