3,3-Diethoxy-1-propyne

Other names:	1-Propyne, 3,3-diethoxy- Propargylaldehyde diethyl acetal 3,3-diethoxypropyne
Inchi:	InChI=1S/C7H12O2/c1-4-7(8-5-2)9-6-3/h1,7H,5-6H2,2-3H3
InchiKey:	RGUXEWWHSQGVRZ-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C#CC(OCC)OCC
Mol. weight [g/mol]:	128.17
CAS:	10160-87-9

Physical Properties

Property code	Value	Unit	Source
gf	18.69	kJ/mol	Joback Method
hf	-165.63	kJ/mol	Joback Method
hfus	15.71	kJ/mol	Joback Method
hvap	35.47	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.019		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	394.08	K	Joback Method
tc	574.54	K	Joback Method
tf	245.08	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.68	J/mol×K	394.08	Joback Method
cpg	226.75	J/mol×K	424.16	Joback Method
cpg	236.53	J/mol×K	454.23	Joback Method
cpg	246.02	J/mol×K	484.31	Joback Method
cpg	255.22	J/mol×K	514.39	Joback Method
cpg	264.12	J/mol×K	544.46	Joback Method

cpg	272.72	J/mol×K	574.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	311.00	K	1.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10160879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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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