2-Butyn-1-al diethyl acetal

Other names: 2-Butynyl aldehyde diethyl acetal
Tetrolaldehyde diethyl acetal
Inchi: InChI=1S/C8H14O2/c1-4-7-8(9-5-2)10-6-3/h8H,5-6H2,1-3H3
InchiKey: FKKVKKSEVMQYER-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CC#CC(OCC)OCC
Mol. weight [g/mol]: 142.20
CAS: 2806-97-5

Physical Properties

Property code	Value	Unit	Source
gf	6.84	kJ/mol	Joback Method
hf	-205.87	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	39.99	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.409		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	435.84	K	Joback Method
tc	626.73	K	Joback Method
tf	315.48	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.62	J/mol×K	435.84	Joback Method
cpg	266.52	J/mol×K	467.65	Joback Method
cpg	278.08	J/mol×K	499.47	Joback Method
cpg	289.29	J/mol×K	531.28	Joback Method
cpg	300.15	J/mol×K	563.10	Joback Method
cpg	310.64	J/mol×K	594.91	Joback Method
cpg	320.76	J/mol×K	626.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.00 ± 1.00	K	1.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2806975&Units=SI

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