2-Octyne, 1,1-diethoxy-

Other names: 1,1-diethoxyoct-2-yne
Inchi: InChI=1S/C12H22O2/c1-4-7-8-9-10-11-12(13-5-2)14-6-3/h12H,4-9H2,1-3H3
InchiKey: YKXAYRBNHIHDSI-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCCCCC#CC(OCC)OCC
Mol. weight [g/mol]: 198.30
CAS: 16387-55-6

Physical Properties

Property code	Value	Unit	Source
chl	-7492.30	kJ/mol	NIST Webbook
gf	40.52	kJ/mol	Joback Method
hf	-288.43	kJ/mol	Joback Method
hfl	-374.00 ± 6.00	kJ/mol	NIST Webbook
hfl	443.10	kJ/mol	NIST Webbook
hfus	28.81	kJ/mol	Joback Method
hvap	48.89	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.969		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
tb	527.36	K	Joback Method
tc	710.36	K	Joback Method
tf	360.56	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.15	J/mol×K	527.36	Joback Method
cpg	447.28	J/mol×K	557.86	Joback Method
cpg	462.82	J/mol×K	588.36	Joback Method
cpg	477.77	J/mol×K	618.86	Joback Method
cpg	492.13	J/mol×K	649.36	Joback Method

cpg	505.89	J/mol×K	679.86	Joback Method
cpg	519.07	J/mol×K	710.36	Joback Method

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=C16387556&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume