Dimethylvinylethynylmethanol butyl ether

Inchi: InChI=1S/C11H18O/c1-5-7-9-11(3,4)12-10-8-6-2/h5H,1,6,8,10H2,2-4H3
InchiKey: OUIQSMDXNSJEQD-UHFFFAOYSA-N
Formula: C11H18O
SMILES: C=CC#CC(C)(C)OCCCC
Mol. weight [g/mol]: 166.26
CAS: 819-41-0

Physical Properties

Property code	Value	Unit	Source
chl	-6836.00 ± 1.30	kJ/mol	NIST Webbook
gf	230.22	kJ/mol	Joback Method
hf	-6.70 ± 1.40	kJ/mol	NIST Webbook
hfl	-62.40 ± 1.40	kJ/mol	NIST Webbook
hfus	19.86	kJ/mol	Joback Method
hvap	55.70	kJ/mol	NIST Webbook
hvap	55.70 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.771		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	475.95	K	Joback Method
tc	673.47	K	Joback Method
tf	342.72	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.77	J/mol×K	475.95	Joback Method
cpg	358.61	J/mol×K	508.87	Joback Method
cpg	373.66	J/mol×K	541.79	Joback Method
cpg	387.95	J/mol×K	574.71	Joback Method
cpg	401.51	J/mol×K	607.63	Joback Method
cpg	414.37	J/mol×K	640.55	Joback Method

cpg	426.55	J/mol×K	673.47	Joback Method

Sources

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=C819410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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