(E)(1-Propenyl) (2-methyl-1-propenyl)ether

Inchi: InChI=1S/C7H12O/c1-4-5-8-6-7(2)3/h4-6H,1-3H3/b5-4+
InchiKey: NDZRKZPGKAYWFD-SNAWJCMRSA-N
Formula: C7H12O
SMILES: CC=COC=C(C)C
Mol. weight [g/mol]: 112.17
CAS: 40716-31-2

Physical Properties

Property code	Value	Unit	Source
gf	54.95	kJ/mol	Joback Method
hf	-95.38	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	33.58	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.460		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	390.18	K	Joback Method
tc	575.76	K	Joback Method
tf	166.76	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.30	J/mol×K	390.18	Joback Method
cpg	200.57	J/mol×K	421.11	Joback Method
cpg	211.32	J/mol×K	452.04	Joback Method
cpg	221.58	J/mol×K	482.97	Joback Method
cpg	231.35	J/mol×K	513.90	Joback Method
cpg	240.66	J/mol×K	544.83	Joback Method
cpg	249.53	J/mol×K	575.76	Joback Method

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=C40716312&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume