

Prop-2-ynyl (E)-2-methylbut-2-enoate

Inchi:	InChI=1S/C8H10O2/c1-4-6-10-8(9)7(3)5-2/h1,5H,6H2,2-3H3/b7-5+
InchiKey:	IOODRSZMVRTKBM-FNORWQNLSA-N
Formula:	C8H10O2
SMILES:	C#CCOC(=O)C(C)=CC
Mol. weight [g/mol]:	138.16

Physical Properties

Property code	Value	Unit	Source
gf	77.30	kJ/mol	Joback Method
hf	-53.92	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.129		Crippen Method
mcvol	118.120	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	1042.00		NIST Webbook
tb	452.89	K	Joback Method
tc	653.15	K	Joback Method
tf	280.01	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.05	J/mol×K	452.89	Joback Method
cpg	243.56	J/mol×K	486.27	Joback Method
cpg	253.56	J/mol×K	519.64	Joback Method
cpg	263.04	J/mol×K	553.02	Joback Method
cpg	272.04	J/mol×K	586.40	Joback Method
cpg	280.58	J/mol×K	619.77	Joback Method
cpg	288.66	J/mol×K	653.15	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=U373725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/35-874-3/Prop-2-ynyl-E-2-methylbut-2-enoate.pdf>

Generated by Cheméo on 2024-04-19 14:44:10.968185852 +0000 UTC m=+15827099.888763173.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.