3-Methyl-2-butenoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C10H12O2/c1-4-5-6-7-12-10(11)8-9(2)3/h1,5-6,8H,7H2,2-3H3
InchiKey: IXQNRTKWPPHICU-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: C#CC=CCOC(=O)C=C(C)C
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	174.36	kJ/mol	Joback Method
hf	22.02	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	46.86	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.685		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	502.81	K	Joback Method
tc	707.33	K	Joback Method
tf	297.47	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.53	J/mol×K	502.81	Joback Method
cpg	310.77	J/mol×K	536.90	Joback Method
cpg	322.31	J/mol×K	570.98	Joback Method
cpg	333.20	J/mol×K	605.07	Joback Method
cpg	343.46	J/mol×K	639.16	Joback Method
cpg	353.14	J/mol×K	673.24	Joback Method
cpg	362.27	J/mol×K	707.33	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=U299310&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