Butanoic acid, 2-propynyl ester

Inchi: InChI=1S/C7H10O2/c1-3-5-7(8)9-6-4-2/h2H,3,5-6H2,1H3
InchiKey: JADOFECNZGDUSZ-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: C#CCOC(=O)CCC
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
gf	-2.79	kJ/mol	Joback Method
hf	-140.71	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	0.963		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
tb	425.97	K	Joback Method
tc	614.89	K	Joback Method
tf	287.78	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.77	J/mol×K	425.97	Joback Method
cpg	220.28	J/mol×K	457.46	Joback Method
cpg	229.42	J/mol×K	488.94	Joback Method
cpg	238.20	J/mol×K	520.43	Joback Method
cpg	246.62	J/mol×K	551.91	Joback Method
cpg	254.68	J/mol×K	583.40	Joback Method

cpg	262.39	J/mol×K	614.89	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=R28693&Units=SI

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