Butanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C10H16O2/c1-4-7-9(6-3)12-10(11)8-5-2/h9H,5-6,8H2,1-3H3
InchiKey: BKDKCQUMBIYJKJ-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC#CC(CC)OC(=O)CCC
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-0.24	kJ/mol	Joback Method
hf	-227.51	kJ/mol	Joback Method
hfus	24.04	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.132		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	997.00		NIST Webbook
tb	513.05	K	Joback Method
tc	710.83	K	Joback Method
tf	365.72	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.95	J/mol×K	513.05	Joback Method
cpg	348.73	J/mol×K	546.01	Joback Method
cpg	361.95	J/mol×K	578.98	Joback Method
cpg	374.59	J/mol×K	611.94	Joback Method
cpg	386.66	J/mol×K	644.91	Joback Method
cpg	398.18	J/mol×K	677.87	Joback Method
cpg	409.14	J/mol×K	710.83	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=U299120&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume