Butanoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C13H22O2/c1-5-7-9-12(10-11(3)4)15-13(14)8-6-2/h11-12H,5-6,8,10H2,1-4H3
InchiKey: PGGRYTIUNQVTQV-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CCC#CC(CC(C)C)OC(=O)CCC
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	22.58	kJ/mol	Joback Method
hf	-294.71	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.158		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1348.00		NIST Webbook
tb	581.25	K	Joback Method
tc	775.23	K	Joback Method
tf	384.53	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.22	J/mol×K	581.25	Joback Method
cpg	494.78	J/mol×K	613.58	Joback Method
cpg	510.59	J/mol×K	645.91	Joback Method
cpg	525.65	J/mol×K	678.24	Joback Method
cpg	539.97	J/mol×K	710.57	Joback Method
cpg	553.58	J/mol×K	742.90	Joback Method
cpg	566.48	J/mol×K	775.23	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=U299122&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