Butanoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C17H30O2/c1-3-5-6-7-8-9-10-11-12-13-14-16-19-17(18)15-4-2/h3-12,15-16H2
InchiKey: SLUOGOVTFIUZSK-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCC
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	61.14	kJ/mol	Joback Method
hf	-366.71	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.864		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook
tb	673.65	K	Joback Method
tc	854.51	K	Joback Method
tf	459.61	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.31	J/mol×K	673.65	Joback Method
cpg	708.20	J/mol×K	703.79	Joback Method
cpg	725.26	J/mol×K	733.94	Joback Method
cpg	741.52	J/mol×K	764.08	Joback Method
cpg	756.98	J/mol×K	794.22	Joback Method
cpg	771.67	J/mol×K	824.37	Joback Method
cpg	785.60	J/mol×K	854.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299126&Units=SI
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

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