Sebacic acid, but-3-yn-2-yl propyl ester

Inchi: InChI=1S/C17H28O4/c1-4-14-20-16(18)12-10-8-6-7-9-11-13-17(19)21-15(3)5-2/h2,15H,4
InchiKey: TVZBRIMJCAVTCJ-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-154.95	kJ/mol	Joback Method
hf	-597.19	kJ/mol	Joback Method
hfus	44.81	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.625		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2007.00		NIST Webbook
tb	730.62	K	Joback Method
tc	914.77	K	Joback Method
tf	457.64	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.13	J/mol×K	730.62	Joback Method
cpg	756.35	J/mol×K	761.31	Joback Method
cpg	771.70	J/mol×K	792.00	Joback Method
cpg	786.22	J/mol×K	822.70	Joback Method
cpg	799.90	J/mol×K	853.39	Joback Method
cpg	812.77	J/mol×K	884.08	Joback Method
cpg	824.84	J/mol×K	914.77	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=U355843&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