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

Inchi: InChI=1S/C18H30O4/c1-5-16(4)22-18(20)13-11-9-7-6-8-10-12-17(19)21-14-15(2)3/h1,15

InchiKey: VJGGKCSEEFNQRZ-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-148.97	kJ/mol	Joback Method
hf	-623.11	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.871		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2067.00		NIST Webbook
tb	753.06	K	Joback Method
tc	939.36	K	Joback Method
tf	453.91	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.68	J/mol×K	753.06	Joback Method
cpg	814.46	J/mol×K	784.11	Joback Method
cpg	830.31	J/mol×K	815.16	Joback Method
cpg	845.24	J/mol×K	846.21	Joback Method
cpg	859.29	J/mol×K	877.26	Joback Method
cpg	872.46	J/mol×K	908.31	Joback Method
cpg	884.77	J/mol×K	939.36	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=U355844&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