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

Inchi: InChI=1S/C19H32O4/c1-4-6-13-16-22-18(20)14-11-9-7-8-10-12-15-19(21)23-17(3)5-2/h2
InchiKey: LMPOTNXOFUMTCJ-UHFFFAOYSA-N
Formula: C19H32O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-138.11	kJ/mol	Joback Method
hf	-638.47	kJ/mol	Joback Method
hfus	49.99	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.405		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2199.00		NIST Webbook
tb	776.38	K	Joback Method
tc	961.54	K	Joback Method
tf	480.18	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.24	J/mol×K	776.38	Joback Method
cpg	872.19	J/mol×K	807.24	Joback Method
cpg	888.20	J/mol×K	838.10	Joback Method
cpg	903.28	J/mol×K	868.96	Joback Method
cpg	917.45	J/mol×K	899.82	Joback Method
cpg	930.74	J/mol×K	930.68	Joback Method
cpg	943.16	J/mol×K	961.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355846&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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