Sebacic acid, hex-4-yn-3-yl propyl ester

Inchi: InChI=1S/C19H32O4/c1-4-13-17(6-3)23-19(21)15-12-10-8-7-9-11-14-18(20)22-16-5-2/h1
InchiKey: RBBOWRZYKXNPIH-UHFFFAOYSA-N
Formula: C19H32O4
SMILES: CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-158.38	kJ/mol	Joback Method
hf	-658.07	kJ/mol	Joback Method
hfus	50.14	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.405		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	795.26	K	Joback Method
tc	986.26	K	Joback Method
tf	539.31	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.94	J/mol×K	795.26	Joback Method
cpg	878.11	J/mol×K	827.09	Joback Method
cpg	894.26	J/mol×K	858.93	Joback Method
cpg	909.41	J/mol×K	890.76	Joback Method
cpg	923.58	J/mol×K	922.59	Joback Method
cpg	936.78	J/mol×K	954.42	Joback Method
cpg	949.02	J/mol×K	986.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355820&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