Sebacic acid, di(hex-4-yn-3-yl) ester

Inchi: InChI=1S/C22H34O4/c1-5-15-19(7-3)25-21(23)17-13-11-9-10-12-14-18-22(24)26-20(8-4
InchiKey: QQLNDMMAGCZRSB-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CC#CC(CC)OC(=O)CCCCCCCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	67.24	kJ/mol	Joback Method
hf	-452.97	kJ/mol	Joback Method
hfus	57.51	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	4.797		Crippen Method
mcvol	318.520	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	2517.00		NIST Webbook
tb	872.46	K	Joback Method
tc	1078.06	K	Joback Method
tf	664.22	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.98	J/mol×K	872.46	Joback Method
cpg	1007.27	J/mol×K	906.73	Joback Method
cpg	1023.33	J/mol×K	940.99	Joback Method
cpg	1038.20	J/mol×K	975.26	Joback Method
cpg	1051.89	J/mol×K	1009.52	Joback Method
cpg	1064.42	J/mol×K	1043.79	Joback Method
cpg	1075.80	J/mol×K	1078.06	Joback Method

Sources

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=U355833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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