Succinic acid, hex-4-yn-3-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C22H34O4/c1-4-7-8-9-10-11-12-13-14-15-19-25-21(23)17-18-22(24)26-20(6-3
InchiKey: SGUHSALCKRMBGJ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CC#CC(CC)OC(=O)CCC(=O)OCCCCCCCCCC#CCC
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	69.68	kJ/mol	Joback Method
hf	-447.69	kJ/mol	Joback Method
hfus	61.03	kJ/mol	Joback Method
hvap	86.79	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.799		Crippen Method
mcvol	318.520	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	872.90	K	Joback Method
tc	1076.99	K	Joback Method
tf	679.22	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.50	J/mol×K	872.90	Joback Method
cpg	1006.68	J/mol×K	906.91	Joback Method
cpg	1022.67	J/mol×K	940.93	Joback Method
cpg	1037.48	J/mol×K	974.94	Joback Method
cpg	1051.15	J/mol×K	1008.96	Joback Method
cpg	1063.69	J/mol×K	1042.97	Joback Method
cpg	1075.11	J/mol×K	1076.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390999&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