Succinic acid, tridec-2-yn-1-yl but-3-en-1-yl ester

Inchi: InChI=1S/C21H34O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-25-21(23)17-16-20(22)24-18-6
InchiKey: USUISHYOGIAJQX-UHFFFAOYSA-N
Formula: C21H34O4
SMILES: C=CCCOC(=O)CCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-51.26	kJ/mol	Joback Method
hf	-568.64	kJ/mol	Joback Method
hfus	57.56	kJ/mol	Joback Method
hvap	82.13	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.963		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	838.14	K	Joback Method
tc	1031.62	K	Joback Method
tf	575.09	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.49	J/mol×K	838.14	Joback Method
cpg	969.65	J/mol×K	870.39	Joback Method
cpg	985.74	J/mol×K	902.63	Joback Method
cpg	1000.81	J/mol×K	934.88	Joback Method
cpg	1014.85	J/mol×K	967.13	Joback Method
cpg	1027.90	J/mol×K	999.37	Joback Method
cpg	1039.98	J/mol×K	1031.62	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=U391204&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