

Succinic acid, tridec-2-yn-1-yl but-2-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:	MKTYYSMDIFDHNX-GQCTYLIASA-N
Formula:	C21H34O4
SMILES:	CC=CCOC(=O)CCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]:	350.49

Physical Properties

Property code	Value	Unit	Source
gf	-58.88	kJ/mol	Joback Method
hf	-576.85	kJ/mol	Joback Method
hfus	59.04	kJ/mol	Joback Method
hvap	82.76	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.963		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	845.62	K	Joback Method
tc	1041.38	K	Joback Method
tf	571.77	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.81	J/mol×K	845.62	Joback Method
cpg	970.97	J/mol×K	878.25	Joback Method
cpg	987.10	J/mol×K	910.87	Joback Method
cpg	1002.21	J/mol×K	943.50	Joback Method
cpg	1016.34	J/mol×K	976.13	Joback Method
cpg	1029.52	J/mol×K	1008.75	Joback Method
cpg	1041.76	J/mol×K	1041.38	Joback Method

Sources

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=U391231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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