Succinic acid, tridec-2-yn-1-yl 2-methoxyethyl ester

Inchi: InChI=1S/C20H34O5/c1-3-4-5-6-7-8-9-10-11-12-13-16-24-19(21)14-15-20(22)25-18-17-2

InchiKey: JYLHQPOKHROYDH-UHFFFAOYSA-N

Formula: C20H34O5

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OCCOC

Mol. weight [g/mol]: 354.48

Physical Properties

Property code	Value	Unit	Source
gf	-252.52	kJ/mol	Joback Method
hf	-805.65	kJ/mol	Joback Method
hfus	57.44	kJ/mol	Joback Method
hvap	82.99	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.034		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	841.00	K	Joback Method
tc	1034.07	K	Joback Method
tf	587.81	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.40	J/mol×K	841.00	Joback Method
cpg	967.40	J/mol×K	873.18	Joback Method
cpg	983.29	J/mol×K	905.36	Joback Method
cpg	998.06	J/mol×K	937.54	Joback Method
cpg	1011.72	J/mol×K	969.71	Joback Method
cpg	1024.27	J/mol×K	1001.89	Joback Method
cpg	1035.73	J/mol×K	1034.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390751&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