Succinic acid, tridec-2-yn-1-yl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C24H40O4/c1-3-4-5-6-7-8-9-10-11-12-13-20-27-23(25)18-19-24(26)28-22-16-1

InchiKey: NSRULGOTUPNZFY-UHFFFAOYSA-N

Formula: C24H40O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-97.10	kJ/mol	Joback Method
hf	-722.01	kJ/mol	Joback Method
hfus	59.52	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.966		Crippen Method
mcvol	344.440	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	924.98	K	Joback Method
tc	1135.84	K	Joback Method
tf	613.80	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.27	J/mol×K	924.98	Joback Method
cpg	1183.93	J/mol×K	960.12	Joback Method
cpg	1200.99	J/mol×K	995.27	Joback Method
cpg	1216.47	J/mol×K	1030.41	Joback Method
cpg	1230.41	J/mol×K	1065.55	Joback Method
cpg	1242.84	J/mol×K	1100.70	Joback Method
cpg	1253.78	J/mol×K	1135.84	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=U390074&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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