Succinic acid, cyclohexylmethyl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C22H34O4/c1-5-9-18(4)20(13-12-17(2)3)26-22(24)15-14-21(23)25-16-19-10-7

InchiKey: XOEUXNRCLOQVMP-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: C=C(C)C#CC(OC(=O)CCC(=O)OCC1CCCCC1)C(C)CCC

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-31.82	kJ/mol	Joback Method
hf	-555.31	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	84.09	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.818		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	879.57	K	Joback Method
tc	1094.28	K	Joback Method
tf	549.78	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.74	J/mol×K	879.57	Joback Method
cpg	1028.08	J/mol×K	915.36	Joback Method
cpg	1044.93	J/mol×K	951.14	Joback Method
cpg	1060.34	J/mol×K	986.93	Joback Method
cpg	1074.34	J/mol×K	1022.71	Joback Method
cpg	1086.97	J/mol×K	1058.50	Joback Method
cpg	1098.26	J/mol×K	1094.28	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=U391017&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