Succinic acid, cyclohexylmethyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C23H38O4/c1-2-3-4-5-6-7-8-9-10-14-19-26-22(24)17-18-23(25)27-20-21-15-12

InchiKey: TZQGZLNNKCTVNK-UHFFFAOYSA-N

Formula: C23H38O4

SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-97.81	kJ/mol	Joback Method
hf	-681.03	kJ/mol	Joback Method
hfus	55.86	kJ/mol	Joback Method
hvap	87.69	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.577		Crippen Method
mcvol	330.350	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	906.77	K	Joback Method
tc	1116.06	K	Joback Method
tf	606.77	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.14	J/mol×K	906.77	Joback Method
cpg	1117.50	J/mol×K	941.65	Joback Method
cpg	1134.37	J/mol×K	976.53	Joback Method
cpg	1149.80	J/mol×K	1011.41	Joback Method
cpg	1163.81	J/mol×K	1046.29	Joback Method
cpg	1176.44	J/mol×K	1081.18	Joback Method
cpg	1187.71	J/mol×K	1116.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391001&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