Succinic acid, hex-4-yn-3-yl 2-naphthyl ester

Inchi: InChI=1S/C20H20O4/c1-3-7-17(4-2)23-19(21)12-13-20(22)24-18-11-10-15-8-5-6-9-16(15

InchiKey: CHSFISYWMDEMKO-UHFFFAOYSA-N

Formula: C20H20O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc2ccccc2c1

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	59.47	kJ/mol	Joback Method
hf	-262.58	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	3.870		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	868.78	K	Joback Method
tc	1101.37	K	Joback Method
tf	622.22	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.34	J/mol×K	868.78	Joback Method
cpg	764.36	J/mol×K	907.55	Joback Method
cpg	777.23	J/mol×K	946.31	Joback Method
cpg	789.00	J/mol×K	985.08	Joback Method
cpg	799.73	J/mol×K	1023.84	Joback Method
cpg	809.48	J/mol×K	1062.61	Joback Method
cpg	818.31	J/mol×K	1101.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389837&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