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

Inchi: InChI=1S/C21H22O4/c1-3-7-19(4-2)25-21(23)13-12-20(22)24-15-16-10-11-17-8-5-6-9-18

InchiKey: SAYBQKRFNYXJFI-UHFFFAOYSA-N

Formula: C21H22O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	67.89	kJ/mol	Joback Method
hf	-283.22	kJ/mol	Joback Method
hfus	45.99	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.008		Crippen Method
mcvol	269.810	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2760.00		NIST Webbook
tb	891.66	K	Joback Method
tc	1121.89	K	Joback Method
tf	633.49	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.74	J/mol×K	891.66	Joback Method
cpg	821.92	J/mol×K	930.03	Joback Method
cpg	834.95	J/mol×K	968.40	Joback Method
cpg	846.87	J/mol×K	1006.78	Joback Method
cpg	857.75	J/mol×K	1045.15	Joback Method
cpg	867.65	J/mol×K	1083.52	Joback Method
cpg	876.62	J/mol×K	1121.89	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=U390001&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