Succinic acid, but-3-yn-2-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C21H20O5/c1-3-16(2)25-21(23)13-12-20(22)24-15-17-8-7-11-19(14-17)26-18-

InchiKey: SSYLUZZXEPAMNQ-UHFFFAOYSA-N

Formula: C21H20O5

SMILES: C#CC(C)OC(=O)CCC(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 352.38

Physical Properties

Property code	Value	Unit	Source
gf	-11.08	kJ/mol	Joback Method
hf	-350.38	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.867		Crippen Method
mcvol	271.380	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2568.00		NIST Webbook
rinpol	2568.00		NIST Webbook
tb	902.90	K	Joback Method
tc	1135.65	K	Joback Method
tf	590.31	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.23	J/mol×K	902.90	Joback Method
cpg	822.18	J/mol×K	941.69	Joback Method
cpg	833.74	J/mol×K	980.48	Joback Method
cpg	843.95	J/mol×K	1019.28	Joback Method
cpg	852.85	J/mol×K	1058.07	Joback Method
cpg	860.48	J/mol×K	1096.86	Joback Method
cpg	866.86	J/mol×K	1135.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390364&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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