Succinic acid, hex-4-yn-3-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H24O5/c1-3-9-19(4-2)28-23(25)15-14-22(24)26-17-18-10-8-13-21(16-18)2

InchiKey: RGNUMXAUHKISDB-UHFFFAOYSA-N

Formula: C23H24O5

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

Mol. weight [g/mol]: 380.43

Physical Properties

Property code	Value	Unit	Source
gf	-14.51	kJ/mol	Joback Method
hf	-411.26	kJ/mol	Joback Method
hfus	49.38	kJ/mol	Joback Method
hvap	94.49	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.647		Crippen Method
mcvol	299.560	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	967.54	K	Joback Method
tc	1204.10	K	Joback Method
tf	671.98	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.21	J/mol×K	967.54	Joback Method
cpg	940.91	J/mol×K	1006.97	Joback Method
cpg	952.03	J/mol×K	1046.39	Joback Method
cpg	961.60	J/mol×K	1085.82	Joback Method
cpg	969.66	J/mol×K	1125.25	Joback Method
cpg	976.23	J/mol×K	1164.68	Joback Method
cpg	981.34	J/mol×K	1204.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390369&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