Succinic acid, hex-4-yn-3-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C17H19BrO5/c1-4-6-13(5-2)22-16(19)9-10-17(20)23-14-8-7-12(18)11-15(14)21

InchiKey: LKGHZLZOHAVYIW-UHFFFAOYSA-N

Formula: C17H19BrO5

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 383.23

Physical Properties

Property code	Value	Unit	Source
gf	-172.75	kJ/mol	Joback Method
hf	-509.09	kJ/mol	Joback Method
hfus	44.70	kJ/mol	Joback Method
hvap	85.96	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.488		Crippen Method
mcvol	256.280	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	874.72	K	Joback Method
tc	1103.75	K	Joback Method
tf	650.26	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.15	J/mol×K	874.72	Joback Method
cpg	729.71	J/mol×K	912.89	Joback Method
cpg	741.04	J/mol×K	951.06	Joback Method
cpg	751.16	J/mol×K	989.23	Joback Method
cpg	760.05	J/mol×K	1027.40	Joback Method
cpg	767.73	J/mol×K	1065.57	Joback Method
cpg	774.17	J/mol×K	1103.75	Joback Method

Sources

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=U390916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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