Succinic acid, but-3-yn-2-yl 4-bromophenyl ester

Inchi: InChI=1S/C14H13BrO4/c1-3-10(2)18-13(16)8-9-14(17)19-12-6-4-11(15)5-7-12/h1,4-7,10

InchiKey: VWFVOZUJAXCPNO-UHFFFAOYSA-N

Formula: C14H13BrO4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 325.15

Physical Properties

Property code	Value	Unit	Source
gf	-63.11	kJ/mol	Joback Method
hf	-283.88	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.700		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	759.80	K	Joback Method
tc	991.79	K	Joback Method
tf	522.57	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.44	J/mol×K	759.80	Joback Method
cpg	539.42	J/mol×K	798.46	Joback Method
cpg	550.45	J/mol×K	837.13	Joback Method
cpg	560.54	J/mol×K	875.79	Joback Method
cpg	569.74	J/mol×K	914.46	Joback Method
cpg	578.05	J/mol×K	953.12	Joback Method
cpg	585.52	J/mol×K	991.79	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=U389819&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