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

Inchi: InChI=1S/C16H17BrO4/c1-3-5-13(4-2)20-15(18)10-11-16(19)21-14-8-6-12(17)7-9-14/h6-
InchiKey: IMRSSGLAQWGJFY-UHFFFAOYSA-N
Formula: C16H17BrO4
SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 353.21

Physical Properties

Property code	Value	Unit	Source
gf	-66.54	kJ/mol	Joback Method
hf	-344.76	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.480		Crippen Method
mcvol	236.320	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	824.44	K	Joback Method
tc	1057.52	K	Joback Method
tf	604.24	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.63	J/mol×K	824.44	Joback Method
cpg	649.63	J/mol×K	863.29	Joback Method
cpg	661.53	J/mol×K	902.13	Joback Method
cpg	672.34	J/mol×K	940.98	Joback Method
cpg	682.09	J/mol×K	979.83	Joback Method
cpg	690.80	J/mol×K	1018.68	Joback Method
cpg	698.50	J/mol×K	1057.52	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=U389823&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

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