Succinic acid, 1-(3-bromophenyl)ethyl ethyl ester

Inchi: InChI=1S/C14H17BrO4/c1-3-18-13(16)7-8-14(17)19-10(2)11-5-4-6-12(15)9-11/h4-6,9-10

InchiKey: RLOCIIFOBSLSSE-UHFFFAOYSA-N

Formula: C14H17BrO4

SMILES: CCOC(=O)CCC(=O)OC(C)c1cccc(Br)c1

Mol. weight [g/mol]: 329.19

Physical Properties

Property code	Value	Unit	Source
gf	-286.18	kJ/mol	Joback Method
hf	-575.78	kJ/mol	Joback Method
hfus	33.00	kJ/mol	Joback Method
hvap	74.06	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.397		Crippen Method
mcvol	216.740	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	769.68	K	Joback Method
tc	989.26	K	Joback Method
tf	475.60	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.31	J/mol×K	769.68	Joback Method
cpg	591.39	J/mol×K	806.28	Joback Method
cpg	603.49	J/mol×K	842.87	Joback Method
cpg	614.62	J/mol×K	879.47	Joback Method
cpg	624.80	J/mol×K	916.07	Joback Method
cpg	634.06	J/mol×K	952.66	Joback Method
cpg	642.40	J/mol×K	989.26	Joback Method
dvisc	0.0007980	Pa×s	475.60	Joback Method

dvisc	0.0004723	Pa×s	524.61	Joback Method
dvisc	0.0003057	Pa×s	573.63	Joback Method
dvisc	0.0002119	Pa×s	622.64	Joback Method
dvisc	0.0001550	Pa×s	671.65	Joback Method
dvisc	0.0001183	Pa×s	720.67	Joback Method
dvisc	0.0000934	Pa×s	769.68	Joback Method

Sources

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=U381461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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