Succinic acid, 1-(3-bromophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H27BrO4/c1-5-7-17(13(2)3)24-19(22)11-10-18(21)23-14(4)15-8-6-9-16(20)

InchiKey: BMOPOIJMYSSEOR-UHFFFAOYSA-N

Formula: C19H27BrO4

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

Mol. weight [g/mol]: 399.32

Physical Properties

Property code	Value	Unit	Source
gf	-248.96	kJ/mol	Joback Method
hf	-689.54	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	84.41	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.201		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	883.20	K	Joback Method
tc	1099.71	K	Joback Method
tf	501.95	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.91	J/mol×K	883.20	Joback Method
cpg	875.47	J/mol×K	919.29	Joback Method
cpg	888.82	J/mol×K	955.37	Joback Method
cpg	901.00	J/mol×K	991.46	Joback Method
cpg	912.04	J/mol×K	1027.54	Joback Method
cpg	921.97	J/mol×K	1063.63	Joback Method
cpg	930.84	J/mol×K	1099.71	Joback Method
dvisc	0.0006056	Pa×s	501.95	Joback Method

dvisc	0.0002948	Pa×s	565.49	Joback Method
dvisc	0.0001659	Pa×s	629.03	Joback Method
dvisc	0.0001038	Pa×s	692.57	Joback Method
dvisc	0.0000703	Pa×s	756.12	Joback Method
dvisc	0.0000505	Pa×s	819.66	Joback Method
dvisc	0.0000381	Pa×s	883.20	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=U381466&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