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

Inchi: InChI=1S/C20H20Br2O4/c1-13(15-5-3-7-17(21)11-15)25-19(23)9-10-20(24)26-14(2)16-6

InchiKey: YCGUSFDMNCRSNM-UHFFFAOYSA-N

Formula: C20H20Br2O4

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

Mol. weight [g/mol]: 484.18

Physical Properties

Property code	Value	Unit	Source
gf	-121.00	kJ/mol	Joback Method
hf	-453.51	kJ/mol	Joback Method
hfus	43.96	kJ/mol	Joback Method
hvap	96.40	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	5.900		Crippen Method
mcvol	295.020	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
tb	1004.34	K	Joback Method
tc	1253.46	K	Joback Method
tf	626.96	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.44	J/mol×K	1004.34	Joback Method
cpg	853.91	J/mol×K	1045.86	Joback Method
cpg	863.14	J/mol×K	1087.38	Joback Method
cpg	871.22	J/mol×K	1128.90	Joback Method
cpg	878.21	J/mol×K	1170.42	Joback Method
cpg	884.19	J/mol×K	1211.94	Joback Method
cpg	889.23	J/mol×K	1253.46	Joback Method
dvisc	0.0002360	Pa×s	626.96	Joback Method

dvisc	0.0001410	Pa×s	689.86	Joback Method
dvisc	0.0000919	Pa×s	752.75	Joback Method
dvisc	0.0000639	Pa×s	815.65	Joback Method
dvisc	0.0000469	Pa×s	878.55	Joback Method
dvisc	0.0000358	Pa×s	941.44	Joback Method
dvisc	0.0000283	Pa×s	1004.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381471&Units=SI
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

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