Succinic acid, 2-bromobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H25BrO4/c1-4-7-16(13(2)3)23-18(21)11-10-17(20)22-12-14-8-5-6-9-15(14)

InchiKey: KBZMSANTBRQQLK-UHFFFAOYSA-N

Formula: C18H25BrO4

SMILES: CCCC(OC(=O)CCC(=O)OCc1ccccc1Br)C(C)C

Mol. weight [g/mol]: 385.29

Physical Properties

Property code	Value	Unit	Source
gf	-254.94	kJ/mol	Joback Method
hf	-663.62	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.640		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	860.76	K	Joback Method
tc	1075.59	K	Joback Method
tf	505.68	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.36	J/mol×K	860.76	Joback Method
cpg	862.65	J/mol×K	1039.78	Joback Method
cpg	852.75	J/mol×K	1003.98	Joback Method
cpg	841.80	J/mol×K	968.17	Joback Method
cpg	829.78	J/mol×K	932.37	Joback Method
cpg	816.64	J/mol×K	896.56	Joback Method
cpg	871.52	J/mol×K	1075.59	Joback Method
dvisc	0.0000484	Pa×s	860.76	Joback Method

dvisc	0.0000630	Pa×s	801.58	Joback Method
dvisc	0.0000856	Pa×s	742.40	Joback Method
dvisc	0.0001227	Pa×s	683.22	Joback Method
dvisc	0.0001883	Pa×s	624.04	Joback Method
dvisc	0.0003161	Pa×s	564.86	Joback Method
dvisc	0.0005989	Pa×s	505.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381120&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

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