Succinic acid, 3-bromobenzyl octyl ester

Inchi: InChI=1S/C19H27BrO4/c1-2-3-4-5-6-7-13-23-18(21)11-12-19(22)24-15-16-9-8-10-17(20)
InchiKey: PAYATLXQWAMZOQ-UHFFFAOYSA-N
Formula: C19H27BrO4
SMILES: CCCCCCCCOC(=O)CCC(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 399.32

Physical Properties

Property code	Value	Unit	Source
gf	-241.64	kJ/mol	Joback Method
hf	-673.70	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.176		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	884.52	K	Joback Method
tc	1095.03	K	Joback Method
tf	546.95	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.35	J/mol×K	884.52	Joback Method
cpg	873.59	J/mol×K	919.60	Joback Method
cpg	886.72	J/mol×K	954.69	Joback Method
cpg	898.78	J/mol×K	989.77	Joback Method
cpg	909.80	J/mol×K	1024.86	Joback Method
cpg	919.80	J/mol×K	1059.94	Joback Method
cpg	928.82	J/mol×K	1095.03	Joback Method
dvisc	0.0004342	Pa×s	546.95	Joback Method

dvisc	0.0002558	Pa×s	603.21	Joback Method
dvisc	0.0001649	Pa×s	659.47	Joback Method
dvisc	0.0001139	Pa×s	715.73	Joback Method
dvisc	0.0000831	Pa×s	772.00	Joback Method
dvisc	0.0000632	Pa×s	828.26	Joback Method
dvisc	0.0000498	Pa×s	884.52	Joback Method

Sources

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=U382420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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