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

Inchi: InChI=1S/C19H27BrO4/c1-3-4-5-6-7-13-23-18(21)11-12-19(22)24-15(2)16-9-8-10-17(20)

InchiKey: GCOMUWPXEHSMJE-UHFFFAOYSA-N

Formula: C19H27BrO4

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

Mol. weight [g/mol]: 399.32

Physical Properties

Property code	Value	Unit	Source
gf	-244.08	kJ/mol	Joback Method
hf	-678.98	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.347		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	884.08	K	Joback Method
tc	1096.44	K	Joback Method
tf	531.95	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.87	J/mol×K	884.08	Joback Method
cpg	920.50	J/mol×K	1061.04	Joback Method
cpg	910.52	J/mol×K	1025.65	Joback Method
cpg	899.50	J/mol×K	990.26	Joback Method
cpg	887.40	J/mol×K	954.87	Joback Method
cpg	874.21	J/mol×K	919.47	Joback Method
cpg	929.47	J/mol×K	1096.44	Joback Method
dvisc	0.0000456	Pa×s	884.08	Joback Method

dvisc	0.0000586	Pa×s	825.39	Joback Method
dvisc	0.0000785	Pa×s	766.70	Joback Method
dvisc	0.0001102	Pa×s	708.01	Joback Method
dvisc	0.0001646	Pa×s	649.33	Joback Method
dvisc	0.0002661	Pa×s	590.64	Joback Method
dvisc	0.0004785	Pa×s	531.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381468&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