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

Inchi: InChI=1S/C18H25BrO4/c1-3-4-5-6-12-22-17(20)10-11-18(21)23-14(2)15-8-7-9-16(19)13-

InchiKey: FWYGWVQJCZZGHF-UHFFFAOYSA-N

Formula: C18H25BrO4

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

Mol. weight [g/mol]: 385.29

Physical Properties

Property code	Value	Unit	Source
gf	-252.50	kJ/mol	Joback Method
hf	-658.34	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.957		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	861.20	K	Joback Method
tc	1073.69	K	Joback Method
tf	520.68	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.82	J/mol×K	861.20	Joback Method
cpg	861.79	J/mol×K	1038.28	Joback Method
cpg	851.89	J/mol×K	1002.86	Joback Method
cpg	840.97	J/mol×K	967.45	Joback Method
cpg	829.00	J/mol×K	932.03	Joback Method
cpg	815.96	J/mol×K	896.62	Joback Method
cpg	870.71	J/mol×K	1073.69	Joback Method
dvisc	0.0000528	Pa×s	861.20	Joback Method

dvisc	0.0000678	Pa×s	804.45	Joback Method
dvisc	0.0000904	Pa×s	747.69	Joback Method
dvisc	0.0001263	Pa×s	690.94	Joback Method
dvisc	0.0001875	Pa×s	634.19	Joback Method
dvisc	0.0003006	Pa×s	577.43	Joback Method
dvisc	0.0005342	Pa×s	520.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381467&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