Succinic acid, 3-bromophenethyl isobutyl ester

Inchi: InChI=1S/C16H21BrO4/c1-12(2)11-21-16(19)7-6-15(18)20-9-8-13-4-3-5-14(17)10-13/h3-

InchiKey: YFWZSEBVYTXVRS-UHFFFAOYSA-N

Formula: C16H21BrO4

SMILES: CC(C)COC(=O)CCC(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 357.24

Physical Properties

Property code	Value	Unit	Source
gf	-269.34	kJ/mol	Joback Method
hf	-617.06	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.514		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	815.44	K	Joback Method
tc	1030.25	K	Joback Method
tf	498.14	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.18	J/mol×K	815.44	Joback Method
cpg	746.45	J/mol×K	994.45	Joback Method
cpg	736.79	J/mol×K	958.65	Joback Method
cpg	726.16	J/mol×K	922.85	Joback Method
cpg	714.53	J/mol×K	887.04	Joback Method
cpg	701.88	J/mol×K	851.24	Joback Method
cpg	755.17	J/mol×K	1030.25	Joback Method
dvisc	0.0000706	Pa×s	815.44	Joback Method

dvisc	0.0000900	Pa×s	762.56	Joback Method
dvisc	0.0001191	Pa×s	709.67	Joback Method
dvisc	0.0001647	Pa×s	656.79	Joback Method
dvisc	0.0002410	Pa×s	603.91	Joback Method
dvisc	0.0003796	Pa×s	551.02	Joback Method
dvisc	0.0006585	Pa×s	498.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381280&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