Succinic acid, 2-methylpent-3-yl 4-bromophenyl ester

Inchi: InChI=1S/C16H21BrO4/c1-4-14(11(2)3)21-16(19)10-9-15(18)20-13-7-5-12(17)6-8-13/h5-

InchiKey: PUZUIGIGHKFHIC-UHFFFAOYSA-N

Formula: C16H21BrO4

SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(Br)cc1)C(C)C

Mol. weight [g/mol]: 357.24

Physical Properties

Property code	Value	Unit	Source
gf	-271.78	kJ/mol	Joback Method
hf	-622.34	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.112		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	815.00	K	Joback Method
tc	1032.80	K	Joback Method
tf	483.14	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.76	J/mol×K	815.00	Joback Method
cpg	702.63	J/mol×K	851.30	Joback Method
cpg	715.42	J/mol×K	887.60	Joback Method
cpg	727.15	J/mol×K	923.90	Joback Method
cpg	737.84	J/mol×K	960.20	Joback Method
cpg	747.52	J/mol×K	996.50	Joback Method
cpg	756.22	J/mol×K	1032.80	Joback Method
dvisc	0.0007442	Pa×s	483.14	Joback Method

dvisc	0.0004021	Pa×s	538.45	Joback Method
dvisc	0.0002436	Pa×s	593.76	Joback Method
dvisc	0.0001608	Pa×s	649.07	Joback Method
dvisc	0.0001132	Pa×s	704.38	Joback Method
dvisc	0.0000839	Pa×s	759.69	Joback Method
dvisc	0.0000648	Pa×s	815.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389821&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