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

Inchi: InChI=1S/C15H19BrO4/c1-10(2)11(3)19-14(17)8-9-15(18)20-13-6-4-12(16)5-7-13/h4-7,1

InchiKey: KODHGOVNMGFQSV-UHFFFAOYSA-N

Formula: C15H19BrO4

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

Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-280.20	kJ/mol	Joback Method
hf	-601.70	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.722		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	792.12	K	Joback Method
tc	1012.33	K	Joback Method
tf	471.87	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.32	J/mol×K	792.12	Joback Method
cpg	691.03	J/mol×K	975.63	Joback Method
cpg	681.52	J/mol×K	938.93	Joback Method
cpg	671.01	J/mol×K	902.23	Joback Method
cpg	659.49	J/mol×K	865.52	Joback Method
cpg	646.93	J/mol×K	828.82	Joback Method
cpg	699.58	J/mol×K	1012.33	Joback Method
dvisc	0.0000748	Pa×s	792.12	Joback Method

dvisc	0.0000965	Pa×s	738.75	Joback Method
dvisc	0.0001297	Pa×s	685.37	Joback Method
dvisc	0.0001832	Pa×s	632.00	Joback Method
dvisc	0.0002757	Pa×s	578.62	Joback Method
dvisc	0.0004510	Pa×s	525.25	Joback Method
dvisc	0.0008246	Pa×s	471.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389820&Units=SI

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