Succinic acid, 3-bromobenzyl isobutyl ester

Inchi: InChI=1S/C15H19BrO4/c1-11(2)9-19-14(17)6-7-15(18)20-10-12-4-3-5-13(16)8-12/h3-5,8
InchiKey: DPFGBOWBKKMXRZ-UHFFFAOYSA-N
Formula: C15H19BrO4
SMILES: CC(C)COC(=O)CCC(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-277.76	kJ/mol	Joback Method
hf	-596.42	kJ/mol	Joback Method
hfus	35.59	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.472		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	792.56	K	Joback Method
tc	1009.47	K	Joback Method
tf	486.87	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.74	J/mol×K	792.56	Joback Method
cpg	646.15	J/mol×K	828.71	Joback Method
cpg	658.55	J/mol×K	864.86	Joback Method
cpg	669.96	J/mol×K	901.02	Joback Method
cpg	680.39	J/mol×K	937.17	Joback Method
cpg	689.87	J/mol×K	973.32	Joback Method
cpg	698.43	J/mol×K	1009.47	Joback Method
dvisc	0.0007265	Pa×s	486.87	Joback Method
dvisc	0.0004243	Pa×s	537.82	Joback Method

dvisc	0.0002720	Pa×s	588.77	Joback Method
dvisc	0.0001871	Pa×s	639.71	Joback Method
dvisc	0.0001361	Pa×s	690.66	Joback Method
dvisc	0.0001033	Pa×s	741.61	Joback Method
dvisc	0.0000813	Pa×s	792.56	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=U382414&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