Succinic acid, 3-bromobenzyl butyl ester

Inchi: InChI=1S/C15H19BrO4/c1-2-3-9-19-14(17)7-8-15(18)20-11-12-5-4-6-13(16)10-12/h4-6,1
InchiKey: YRZYNOQGUMACLN-UHFFFAOYSA-N
Formula: C15H19BrO4
SMILES: CCCCOC(=O)CCC(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-275.32	kJ/mol	Joback Method
hf	-591.14	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.616		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	793.00	K	Joback Method
tc	1006.77	K	Joback Method
tf	501.87	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.16	J/mol×K	793.00	Joback Method
cpg	645.38	J/mol×K	828.63	Joback Method
cpg	657.63	J/mol×K	864.26	Joback Method
cpg	668.93	J/mol×K	899.88	Joback Method
cpg	679.29	J/mol×K	935.51	Joback Method
cpg	688.74	J/mol×K	971.14	Joback Method
cpg	697.29	J/mol×K	1006.77	Joback Method
dvisc	0.0006502	Pa×s	501.87	Joback Method

dvisc	0.0004028	Pa×s	550.39	Joback Method
dvisc	0.0002696	Pa×s	598.91	Joback Method
dvisc	0.0001917	Pa×s	647.43	Joback Method
dvisc	0.0001429	Pa×s	695.96	Joback Method
dvisc	0.0001107	Pa×s	744.48	Joback Method
dvisc	0.0000885	Pa×s	793.00	Joback Method

Sources

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=U382415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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