Succinic acid, 5-bromo-2-methoxybenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H27BrO5/c1-5-6-16(13(2)3)25-19(22)10-9-18(21)24-12-14-11-15(20)7-8-17

InchiKey: ANVGYEQLPHJOIC-UHFFFAOYSA-N

Formula: C19H27BrO5

SMILES: CCCC(OC(=O)CCC(=O)OCc1cc(Br)ccc1OC)C(C)C

Mol. weight [g/mol]: 415.32

Physical Properties

Property code	Value	Unit	Source
gf	-361.15	kJ/mol	Joback Method
hf	-827.95	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.649		Crippen Method
mcvol	293.060	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	911.04	K	Joback Method
tc	1126.94	K	Joback Method
tf	551.70	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.11	J/mol×K	911.04	Joback Method
cpg	900.81	J/mol×K	947.02	Joback Method
cpg	913.22	J/mol×K	983.01	Joback Method
cpg	924.35	J/mol×K	1018.99	Joback Method
cpg	934.22	J/mol×K	1054.98	Joback Method
cpg	942.84	J/mol×K	1090.96	Joback Method
cpg	950.22	J/mol×K	1126.94	Joback Method
dvisc	0.0003204	Pa×s	551.70	Joback Method

dvisc	0.0001800	Pa×s	611.59	Joback Method
dvisc	0.0001120	Pa×s	671.48	Joback Method
dvisc	0.0000754	Pa×s	731.37	Joback Method
dvisc	0.0000539	Pa×s	791.26	Joback Method
dvisc	0.0000403	Pa×s	851.15	Joback Method
dvisc	0.0000314	Pa×s	911.04	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=U381077&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