Succinic acid, 5-bromo-2-methoxybenzyl isobutyl ester

Inchi: InChI=1S/C16H21BrO5/c1-11(2)9-21-15(18)6-7-16(19)22-10-12-8-13(17)4-5-14(12)20-3/

InchiKey: GSNDJAMQHFHZHB-UHFFFAOYSA-N

Formula: C16H21BrO5

SMILES: COc1ccc(Br)cc1COC(=O)CCC(=O)OCC(C)C

Mol. weight [g/mol]: 373.24

Physical Properties

Property code	Value	Unit	Source
gf	-383.97	kJ/mol	Joback Method
hf	-760.75	kJ/mol	Joback Method
hfus	38.98	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.480		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	842.84	K	Joback Method
tc	1057.61	K	Joback Method
tf	532.89	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.92	J/mol×K	842.84	Joback Method
cpg	768.50	J/mol×K	1021.82	Joback Method
cpg	759.79	J/mol×K	986.02	Joback Method
cpg	749.98	J/mol×K	950.23	Joback Method
cpg	739.06	J/mol×K	914.43	Joback Method
cpg	727.04	J/mol×K	878.64	Joback Method
cpg	776.11	J/mol×K	1057.61	Joback Method
dvisc	0.0000535	Pa×s	842.84	Joback Method

dvisc	0.0000671	Pa×s	791.18	Joback Method
dvisc	0.0000869	Pa×s	739.52	Joback Method
dvisc	0.0001170	Pa×s	687.87	Joback Method
dvisc	0.0001653	Pa×s	636.21	Joback Method
dvisc	0.0002483	Pa×s	584.55	Joback Method
dvisc	0.0004036	Pa×s	532.89	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=U381071&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