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

Inchi: InChI=1S/C16H21BrO5/c1-3-4-9-21-15(18)7-8-16(19)22-11-12-10-13(17)5-6-14(12)20-2/
InchiKey: ONTSINWOGTYNRQ-UHFFFAOYSA-N
Formula: C16H21BrO5
SMILES: CCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]: 373.24

Physical Properties

Property code	Value	Unit	Source
gf	-381.53	kJ/mol	Joback Method
hf	-755.47	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.624		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	843.28	K	Joback Method
tc	1055.51	K	Joback Method
tf	547.89	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.35	J/mol×K	843.28	Joback Method
cpg	767.62	J/mol×K	1020.14	Joback Method
cpg	758.90	J/mol×K	984.77	Joback Method
cpg	749.11	J/mol×K	949.40	Joback Method
cpg	738.26	J/mol×K	914.02	Joback Method
cpg	726.34	J/mol×K	878.65	Joback Method
cpg	775.28	J/mol×K	1055.51	Joback Method
dvisc	0.0000583	Pa×s	843.28	Joback Method

dvisc	0.0000722	Pa×s	794.05	Joback Method
dvisc	0.0000918	Pa×s	744.82	Joback Method
dvisc	0.0001208	Pa×s	695.59	Joback Method
dvisc	0.0001658	Pa×s	646.35	Joback Method
dvisc	0.0002398	Pa×s	597.12	Joback Method
dvisc	0.0003705	Pa×s	547.89	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=U381072&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