Succinic acid, 8-chlorooctyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C19H26BrClO5/c1-24-17-14-15(20)8-9-16(17)26-19(23)11-10-18(22)25-13-7-5

InchiKey: ZYSCYMLLLPFMJI-UHFFFAOYSA-N

Formula: C19H26BrClO5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)OCCCCCCCCCCl

Mol. weight [g/mol]: 449.76

Physical Properties

Property code	Value	Unit	Source
gf	-368.20	kJ/mol	Joback Method
hf	-833.13	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	93.03	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.266		Crippen Method
mcvol	305.300	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	3116.00		NIST Webbook
rinpol	3116.00		NIST Webbook
tb	949.35	K	Joback Method
tc	1167.71	K	Joback Method
tf	611.62	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.04	J/mol×K	949.35	Joback Method
cpg	921.35	J/mol×K	985.74	Joback Method
cpg	932.40	J/mol×K	1022.14	Joback Method
cpg	942.20	J/mol×K	1058.53	Joback Method
cpg	950.77	J/mol×K	1094.93	Joback Method
cpg	958.12	J/mol×K	1131.32	Joback Method
cpg	964.27	J/mol×K	1167.71	Joback Method
dvisc	0.0002220	Pa×s	611.62	Joback Method

dvisc	0.0001400	Pa×s	667.91	Joback Method
dvisc	0.0000949	Pa×s	724.20	Joback Method
dvisc	0.0000680	Pa×s	780.48	Joback Method
dvisc	0.0000510	Pa×s	836.77	Joback Method
dvisc	0.0000396	Pa×s	893.06	Joback Method
dvisc	0.0000317	Pa×s	949.35	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=U390924&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