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

Inchi: InChI=1S/C23H35BrO5/c1-3-4-5-6-7-8-9-10-11-16-28-22(25)14-15-23(26)29-18-19-17-20

InchiKey: DGACCDOPVMBXJB-UHFFFAOYSA-N

Formula: C23H35BrO5

SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 471.43

Physical Properties

Property code	Value	Unit	Source
gf	-322.59	kJ/mol	Joback Method
hf	-899.95	kJ/mol	Joback Method
hfus	60.64	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.355		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	3143.00		NIST Webbook
rinpol	3143.00		NIST Webbook
tb	1003.44	K	Joback Method
tc	1228.50	K	Joback Method
tf	626.78	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.30	J/mol×K	1003.44	Joback Method
cpg	1139.46	J/mol×K	1040.95	Joback Method
cpg	1152.08	J/mol×K	1078.46	Joback Method
cpg	1163.20	J/mol×K	1115.97	Joback Method
cpg	1172.84	J/mol×K	1153.48	Joback Method
cpg	1181.03	J/mol×K	1190.99	Joback Method
cpg	1187.81	J/mol×K	1228.50	Joback Method
dvisc	0.0001712	Pa×s	626.78	Joback Method

dvisc	0.0001022	Pa×s	689.56	Joback Method
dvisc	0.0000665	Pa×s	752.33	Joback Method
dvisc	0.0000463	Pa×s	815.11	Joback Method
dvisc	0.0000339	Pa×s	877.89	Joback Method
dvisc	0.0000259	Pa×s	940.66	Joback Method
dvisc	0.0000204	Pa×s	1003.44	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=U381080&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