Succinic acid, 2-bromophenethyl dodecyl ester

Inchi: InChI=1S/C24H37BrO4/c1-2-3-4-5-6-7-8-9-10-13-19-28-23(26)16-17-24(27)29-20-18-21-
InchiKey: YPEFGEKERGDDOP-UHFFFAOYSA-N
Formula: C24H37BrO4
SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccccc1Br
Mol. weight [g/mol]: 469.45

Physical Properties

Property code	Value	Unit	Source
gf	-199.54	kJ/mol	Joback Method
hf	-776.90	kJ/mol	Joback Method
hfus	62.43	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.779		Crippen Method
mcvol	357.640	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3134.00		NIST Webbook
rinpol	3134.00		NIST Webbook
tb	998.92	K	Joback Method
tc	1222.96	K	Joback Method
tf	603.30	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.59	J/mol×K	998.92	Joback Method
cpg	1174.96	J/mol×K	1036.26	Joback Method
cpg	1188.96	J/mol×K	1073.60	Joback Method
cpg	1201.64	J/mol×K	1110.94	Joback Method
cpg	1213.05	J/mol×K	1148.28	Joback Method
cpg	1223.25	J/mol×K	1185.62	Joback Method
cpg	1232.30	J/mol×K	1222.96	Joback Method
dvisc	0.0002425	Pa×s	603.30	Joback Method

dvisc	0.0001353	Pa×s	669.24	Joback Method
dvisc	0.0000838	Pa×s	735.17	Joback Method
dvisc	0.0000562	Pa×s	801.11	Joback Method
dvisc	0.0000400	Pa×s	867.05	Joback Method
dvisc	0.0000299	Pa×s	932.98	Joback Method
dvisc	0.0000232	Pa×s	998.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U381458&Units=SI

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

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