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

Inchi: InChI=1S/C24H37BrO5/c1-3-4-5-6-7-8-9-10-11-12-17-29-23(26)15-16-24(27)30-19-20-18
InchiKey: PTXAQOOHEUNUKR-UHFFFAOYSA-N
Formula: C24H37BrO5
SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]: 485.45

Physical Properties

Property code	Value	Unit	Source
gf	-314.17	kJ/mol	Joback Method
hf	-920.59	kJ/mol	Joback Method
hfus	63.23	kJ/mol	Joback Method
hvap	99.77	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	6.745		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	3249.00		NIST Webbook
rinpol	3249.00		NIST Webbook
tb	1026.32	K	Joback Method
tc	1256.97	K	Joback Method
tf	638.05	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.27	J/mol×K	1026.32	Joback Method
cpg	1200.58	J/mol×K	1064.76	Joback Method
cpg	1213.25	J/mol×K	1103.20	Joback Method
cpg	1224.31	J/mol×K	1141.65	Joback Method
cpg	1233.80	J/mol×K	1180.09	Joback Method
cpg	1241.75	J/mol×K	1218.53	Joback Method
cpg	1248.21	J/mol×K	1256.97	Joback Method
dvisc	0.0001515	Pa×s	638.05	Joback Method

dvisc	0.0000895	Pa×s	702.76	Joback Method
dvisc	0.0000578	Pa×s	767.47	Joback Method
dvisc	0.0000400	Pa×s	832.18	Joback Method
dvisc	0.0000291	Pa×s	896.90	Joback Method
dvisc	0.0000222	Pa×s	961.61	Joback Method
dvisc	0.0000175	Pa×s	1026.32	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=U381081&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