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

Inchi: InChI=1S/C27H35BrO5/c1-3-4-5-6-7-8-9-10-13-18-32-26(29)23-14-11-12-15-24(23)27(30

InchiKey: LMLMPDQXBKYDFR-UHFFFAOYSA-N

Formula: C27H35BrO5

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 519.47

Physical Properties

Property code	Value	Unit	Source
gf	-186.13	kJ/mol	Joback Method
hf	-757.45	kJ/mol	Joback Method
hfus	64.65	kJ/mol	Joback Method
hvap	109.39	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	7.502		Crippen Method
mcvol	382.020	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	3499.00		NIST Webbook
rinpol	3499.00		NIST Webbook
tb	1126.62	K	Joback Method
tc	1380.13	K	Joback Method
tf	710.80	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.26	J/mol×K	1126.62	Joback Method
cpg	1289.80	J/mol×K	1337.88	Joback Method
cpg	1285.98	J/mol×K	1295.63	Joback Method
cpg	1280.48	J/mol×K	1253.38	Joback Method
cpg	1273.23	J/mol×K	1211.12	Joback Method
cpg	1264.18	J/mol×K	1168.87	Joback Method
cpg	1292.00	J/mol×K	1380.13	Joback Method
dvisc	0.0000117	Pa×s	1126.62	Joback Method

dvisc	0.0000147	Pa×s	1057.32	Joback Method
dvisc	0.0000190	Pa×s	988.01	Joback Method
dvisc	0.0000256	Pa×s	918.71	Joback Method
dvisc	0.0000363	Pa×s	849.41	Joback Method
dvisc	0.0000546	Pa×s	780.10	Joback Method
dvisc	0.0000890	Pa×s	710.80	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=U382873&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