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

Inchi: InChI=1S/C26H33BrO5/c1-3-4-5-6-7-8-9-12-17-31-25(28)22-13-10-11-14-23(22)26(29)32

InchiKey: TVAWJRFUHDIQQA-UHFFFAOYSA-N

Formula: C26H33BrO5

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

Mol. weight [g/mol]: 505.44

Physical Properties

Property code	Value	Unit	Source
gf	-194.55	kJ/mol	Joback Method
hf	-736.81	kJ/mol	Joback Method
hfus	62.06	kJ/mol	Joback Method
hvap	107.16	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	7.112		Crippen Method
mcvol	367.930	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	3398.00		NIST Webbook
rinpol	3398.00		NIST Webbook
tb	1103.74	K	Joback Method
tc	1351.31	K	Joback Method
tf	699.53	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.87	J/mol×K	1103.74	Joback Method
cpg	1203.83	J/mol×K	1145.00	Joback Method
cpg	1213.03	J/mol×K	1186.26	Joback Method
cpg	1220.51	J/mol×K	1227.52	Joback Method
cpg	1226.32	J/mol×K	1268.78	Joback Method
cpg	1230.53	J/mol×K	1310.04	Joback Method
cpg	1233.18	J/mol×K	1351.31	Joback Method
dvisc	0.0001010	Pa×s	699.53	Joback Method

dvisc	0.0000625	Pa×s	766.90	Joback Method
dvisc	0.0000418	Pa×s	834.27	Joback Method
dvisc	0.0000297	Pa×s	901.63	Joback Method
dvisc	0.0000222	Pa×s	969.00	Joback Method
dvisc	0.0000172	Pa×s	1036.37	Joback Method
dvisc	0.0000137	Pa×s	1103.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382872&Units=SI
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

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