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

Inchi: InChI=1S/C25H31BrO5/c1-3-4-5-6-7-8-11-16-30-24(27)21-12-9-10-13-22(21)25(28)31-18

InchiKey: AGRCELSYDNDJMQ-UHFFFAOYSA-N

Formula: C25H31BrO5

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

Mol. weight [g/mol]: 491.42

Physical Properties

Property code	Value	Unit	Source
gf	-202.97	kJ/mol	Joback Method
hf	-716.17	kJ/mol	Joback Method
hfus	59.47	kJ/mol	Joback Method
hvap	104.94	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	6.722		Crippen Method
mcvol	353.840	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	3298.00		NIST Webbook
rinpol	3298.00		NIST Webbook
tb	1080.86	K	Joback Method
tc	1323.67	K	Joback Method
tf	688.26	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.76	J/mol×K	1080.86	Joback Method
cpg	1143.77	J/mol×K	1121.33	Joback Method
cpg	1153.09	J/mol×K	1161.80	Joback Method
cpg	1160.78	J/mol×K	1202.27	Joback Method
cpg	1166.87	J/mol×K	1242.73	Joback Method
cpg	1171.41	J/mol×K	1283.20	Joback Method
cpg	1174.45	J/mol×K	1323.67	Joback Method
dvisc	0.0001142	Pa×s	688.26	Joback Method

dvisc	0.0000714	Pa×s	753.69	Joback Method
dvisc	0.0000482	Pa×s	819.13	Joback Method
dvisc	0.0000344	Pa×s	884.56	Joback Method
dvisc	0.0000258	Pa×s	949.99	Joback Method
dvisc	0.0000200	Pa×s	1015.43	Joback Method
dvisc	0.0000160	Pa×s	1080.86	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=U382871&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