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

Inchi: InChI=1S/C24H29BrO5/c1-3-4-5-6-7-10-15-29-23(26)20-11-8-9-12-21(20)24(27)30-17-18

InchiKey: PYFVECPFQUUPER-UHFFFAOYSA-N

Formula: C24H29BrO5

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

Mol. weight [g/mol]: 477.39

Physical Properties

Property code	Value	Unit	Source
gf	-211.39	kJ/mol	Joback Method
hf	-695.53	kJ/mol	Joback Method
hfus	56.88	kJ/mol	Joback Method
hvap	102.71	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	6.332		Crippen Method
mcvol	339.750	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	1057.98	K	Joback Method
tc	1297.15	K	Joback Method
tf	676.99	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.97	J/mol×K	1057.98	Joback Method
cpg	1084.02	J/mol×K	1097.84	Joback Method
cpg	1093.46	J/mol×K	1137.70	Joback Method
cpg	1101.32	J/mol×K	1177.57	Joback Method
cpg	1107.65	J/mol×K	1217.43	Joback Method
cpg	1112.49	J/mol×K	1257.29	Joback Method
cpg	1115.87	J/mol×K	1297.15	Joback Method
dvisc	0.0001289	Pa×s	676.99	Joback Method

dvisc	0.0000814	Pa×s	740.49	Joback Method
dvisc	0.0000553	Pa×s	803.99	Joback Method
dvisc	0.0000398	Pa×s	867.49	Joback Method
dvisc	0.0000299	Pa×s	930.98	Joback Method
dvisc	0.0000233	Pa×s	994.48	Joback Method
dvisc	0.0000187	Pa×s	1057.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382870&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

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