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

Inchi: InChI=1S/C19H19BrO5/c1-3-10-24-18(21)15-6-4-5-7-16(15)19(22)25-12-13-11-14(20)8-9

InchiKey: ALZIFKWDHZADDD-UHFFFAOYSA-N

Formula: C19H19BrO5

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

Mol. weight [g/mol]: 407.25

Physical Properties

Property code	Value	Unit	Source
gf	-253.49	kJ/mol	Joback Method
hf	-592.33	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.381		Crippen Method
mcvol	269.300	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	2704.00		NIST Webbook
rinpol	2704.00		NIST Webbook
tb	943.58	K	Joback Method
tc	1179.23	K	Joback Method
tf	620.64	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.50	J/mol×K	943.58	Joback Method
cpg	822.33	J/mol×K	1139.96	Joback Method
cpg	816.65	J/mol×K	1100.68	Joback Method
cpg	809.65	J/mol×K	1061.41	Joback Method
cpg	801.30	J/mol×K	1022.13	Joback Method
cpg	791.59	J/mol×K	982.86	Joback Method
cpg	826.70	J/mol×K	1179.23	Joback Method
dvisc	0.0000398	Pa×s	943.58	Joback Method

dvisc	0.0000487	Pa×s	889.76	Joback Method
dvisc	0.0000612	Pa×s	835.93	Joback Method
dvisc	0.0000793	Pa×s	782.11	Joback Method
dvisc	0.0001068	Pa×s	728.29	Joback Method
dvisc	0.0001510	Pa×s	674.46	Joback Method
dvisc	0.0002266	Pa×s	620.64	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=U382864&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