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

Inchi: InChI=1S/C21H23BrO5/c1-3-4-7-12-26-20(23)17-8-5-6-9-18(17)21(24)27-14-15-13-16(22

InchiKey: XQKFFSHAKFEDLZ-UHFFFAOYSA-N

Formula: C21H23BrO5

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

Mol. weight [g/mol]: 435.31

Physical Properties

Property code	Value	Unit	Source
gf	-236.65	kJ/mol	Joback Method
hf	-633.61	kJ/mol	Joback Method
hfus	49.11	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.162		Crippen Method
mcvol	297.480	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	989.34	K	Joback Method
tc	1223.69	K	Joback Method
tf	643.18	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.99	J/mol×K	989.34	Joback Method
cpg	907.12	J/mol×K	1028.40	Joback Method
cpg	916.79	J/mol×K	1067.46	Joback Method
cpg	925.03	J/mol×K	1106.52	Joback Method
cpg	931.87	J/mol×K	1145.57	Joback Method
cpg	937.34	J/mol×K	1184.63	Joback Method
cpg	941.45	J/mol×K	1223.69	Joback Method
dvisc	0.0001824	Pa×s	643.18	Joback Method

dvisc	0.0001189	Pa×s	700.87	Joback Method
dvisc	0.0000827	Pa×s	758.57	Joback Method
dvisc	0.0000606	Pa×s	816.26	Joback Method
dvisc	0.0000462	Pa×s	873.95	Joback Method
dvisc	0.0000365	Pa×s	931.65	Joback Method
dvisc	0.0000296	Pa×s	989.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382867&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