Terephthalic acid, 3-bromobenzyl butyl ester

Inchi: InChI=1S/C19H19BrO4/c1-2-3-11-23-18(21)15-7-9-16(10-8-15)19(22)24-13-14-5-4-6-17(
InchiKey: IOTJGPNDAOOZKE-UHFFFAOYSA-N
Formula: C19H19BrO4
SMILES: CCCCOC(=O)c1ccc(C(=O)OCc2cccc(Br)c2)cc1
Mol. weight [g/mol]: 391.26

Physical Properties

Property code	Value	Unit	Source
gf	-138.86	kJ/mol	Joback Method
hf	-448.64	kJ/mol	Joback Method
hfus	43.13	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.763		Crippen Method
mcvol	263.430	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
tb	916.18	K	Joback Method
tc	1152.18	K	Joback Method
tf	585.89	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.39	J/mol×K	916.18	Joback Method
cpg	768.42	J/mol×K	955.51	Joback Method
cpg	779.21	J/mol×K	994.85	Joback Method
cpg	788.81	J/mol×K	1034.18	Joback Method
cpg	797.27	J/mol×K	1073.52	Joback Method
cpg	804.63	J/mol×K	1112.85	Joback Method
cpg	810.93	J/mol×K	1152.18	Joback Method
dvisc	0.0003492	Pa×s	585.89	Joback Method

dvisc	0.0002222	Pa×s	640.94	Joback Method
dvisc	0.0001518	Pa×s	695.99	Joback Method
dvisc	0.0001097	Pa×s	751.03	Joback Method
dvisc	0.0000829	Pa×s	806.08	Joback Method
dvisc	0.0000649	Pa×s	861.13	Joback Method
dvisc	0.0000523	Pa×s	916.18	Joback Method

Sources

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=U383022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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