Terephthalic acid, 3-bromobenzyl isobutyl ester

Inchi: InChI=1S/C19H19BrO4/c1-13(2)11-23-18(21)15-6-8-16(9-7-15)19(22)24-12-14-4-3-5-17(

InchiKey: NLWDLKAJVBHMOC-UHFFFAOYSA-N

Formula: C19H19BrO4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2cccc(Br)c2)cc1

Mol. weight [g/mol]: 391.26

Physical Properties

Property code	Value	Unit	Source
gf	-141.30	kJ/mol	Joback Method
hf	-453.92	kJ/mol	Joback Method
hfus	39.61	kJ/mol	Joback Method
hvap	88.12	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.619		Crippen Method
mcvol	263.430	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	3168.00		NIST Webbook
rinpol	3168.00		NIST Webbook
tb	915.74	K	Joback Method
tc	1154.83	K	Joback Method
tf	570.89	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.92	J/mol×K	915.74	Joback Method
cpg	805.25	J/mol×K	1114.98	Joback Method
cpg	797.96	J/mol×K	1075.13	Joback Method
cpg	789.53	J/mol×K	1035.28	Joback Method
cpg	779.91	J/mol×K	995.44	Joback Method
cpg	769.05	J/mol×K	955.59	Joback Method
cpg	811.44	J/mol×K	1154.83	Joback Method
dvisc	0.0000478	Pa×s	915.74	Joback Method

dvisc	0.0000600	Pa×s	858.26	Joback Method
dvisc	0.0000779	Pa×s	800.79	Joback Method
dvisc	0.0001053	Pa×s	743.32	Joback Method
dvisc	0.0001498	Pa×s	685.84	Joback Method
dvisc	0.0002272	Pa×s	628.37	Joback Method
dvisc	0.0003747	Pa×s	570.89	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=U383021&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