

Terephthalic acid, 2-bromobenzyl isobutyl ester

Inchi:	InChI=1S/C19H19BrO4/c1-13(2)11-23-18(21)14-7-9-15(10-8-14)19(22)24-12-16-5-3-4-6
InchiKey:	FFNHVURDSWJESG-UHFFFAOYSA-N
Formula:	C19H19BrO4
SMILES:	CC(C)COC(=O)c1ccc(C(=O)OCc2ccccc2Br)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
mvol	263.430	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook
tb	915.74	K	Joback Method
tc	1154.83	K	Joback Method
tf	570.89	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.92	J/molxK	915.74	Joback Method
cpg	769.05	J/molxK	955.59	Joback Method
cpg	779.91	J/molxK	995.44	Joback Method
cpg	789.53	J/molxK	1035.28	Joback Method
cpg	797.96	J/molxK	1075.13	Joback Method
cpg	805.25	J/molxK	1114.98	Joback Method
cpg	811.44	J/molxK	1154.83	Joback Method
dvisc	0.0003747	Paxs	570.89	Joback Method

dvisc	0.0002272	Paxs	628.37	Joback Method
dvisc	0.0001498	Paxs	685.84	Joback Method
dvisc	0.0001053	Paxs	743.32	Joback Method
dvisc	0.0000779	Paxs	800.79	Joback Method
dvisc	0.0000600	Paxs	858.26	Joback Method
dvisc	0.0000478	Paxs	915.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U416079&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

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