Terephthalic acid, 2-bromobenzyl ethyl ester

Inchi: InChI=1S/C17H15BrO4/c1-2-21-16(19)12-7-9-13(10-8-12)17(20)22-11-14-5-3-4-6-15(14)
InchiKey: LRIMYPCPESZUIB-UHFFFAOYSA-N
Formula: C17H15BrO4
SMILES: CCOC(=O)c1ccc(C(=O)OCc2ccccc2Br)cc1
Mol. weight [g/mol]: 363.20

Physical Properties

Property code	Value	Unit	Source
gf	-155.70	kJ/mol	Joback Method
hf	-407.36	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.983		Crippen Method
mcvol	235.250	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook
tb	870.42	K	Joback Method
tc	1112.19	K	Joback Method
tf	563.35	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.96	J/mol×K	870.42	Joback Method
cpg	655.66	J/mol×K	910.71	Joback Method
cpg	666.16	J/mol×K	951.01	Joback Method
cpg	675.49	J/mol×K	991.30	Joback Method
cpg	683.69	J/mol×K	1031.60	Joback Method
cpg	690.80	J/mol×K	1071.89	Joback Method
cpg	696.86	J/mol×K	1112.19	Joback Method
dvisc	0.0004265	Pa×s	563.35	Joback Method

dvisc	0.0002779	Pa×s	614.53	Joback Method
dvisc	0.0001934	Pa×s	665.71	Joback Method
dvisc	0.0001418	Pa×s	716.88	Joback Method
dvisc	0.0001083	Pa×s	768.06	Joback Method
dvisc	0.0000856	Pa×s	819.24	Joback Method
dvisc	0.0000695	Pa×s	870.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416077&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