Isophthalic acid, 4-bromophenyl propyl ester

Inchi: InChI=1S/C17H15BrO4/c1-2-10-21-16(19)12-4-3-5-13(11-12)17(20)22-15-8-6-14(18)7-9-
InchiKey: AYTVUHUVGWUVRX-UHFFFAOYSA-N
Formula: C17H15BrO4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
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	-5.80		Crippen Method
logp	4.235		Crippen Method
mcvol	235.250	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	2689.00		NIST Webbook
rinpol	2689.00		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

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=U344464&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