Phthalic acid, di(2-(3-bromophenyl)ethyl) ester

Inchi: InChI=1S/C24H20Br2O4/c25-19-7-3-5-17(15-19)11-13-29-23(27)21-9-1-2-10-22(21)24(2
InchiKey: GHQNAWSFOAWTPN-UHFFFAOYSA-N
Formula: C24H20Br2O4
SMILES: O=C(OCCc1cccc(Br)c1)c1ccccc1C(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]: 532.22

Physical Properties

Property code	Value	Unit	Source
gf	20.34	kJ/mol	Joback Method
hf	-300.45	kJ/mol	Joback Method
hfus	55.02	kJ/mol	Joback Method
hvap	109.01	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	6.011		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	3632.00		NIST Webbook
rinpol	3632.00		NIST Webbook
tb	1128.40	K	Joback Method
tc	1394.25	K	Joback Method
tf	740.98	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.92	J/mol×K	1128.40	Joback Method
cpg	966.32	J/mol×K	1172.71	Joback Method
cpg	973.56	J/mol×K	1217.02	Joback Method
cpg	979.75	J/mol×K	1261.33	Joback Method
cpg	985.01	J/mol×K	1305.63	Joback Method
cpg	989.45	J/mol×K	1349.94	Joback Method
cpg	993.18	J/mol×K	1394.25	Joback Method
dvisc	0.0001160	Pa×s	740.98	Joback Method

dvisc	0.0000767	Pa×s	805.55	Joback Method
dvisc	0.0000540	Pa×s	870.12	Joback Method
dvisc	0.0000398	Pa×s	934.69	Joback Method
dvisc	0.0000306	Pa×s	999.26	Joback Method
dvisc	0.0000242	Pa×s	1063.83	Joback Method
dvisc	0.0000197	Pa×s	1128.40	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=U378033&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