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

Inchi: InChI=1S/C20H21BrO4/c1-2-3-12-24-19(22)17-9-4-5-10-18(17)20(23)25-13-11-15-7-6-8-

InchiKey: LJYQTHYESFRHHW-UHFFFAOYSA-N

Formula: C20H21BrO4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 405.28

Physical Properties

Property code	Value	Unit	Source
gf	-130.44	kJ/mol	Joback Method
hf	-469.28	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.806		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	939.06	K	Joback Method
tc	1173.28	K	Joback Method
tf	597.16	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.72	J/mol×K	939.06	Joback Method
cpg	825.86	J/mol×K	978.10	Joback Method
cpg	836.75	J/mol×K	1017.13	Joback Method
cpg	846.44	J/mol×K	1056.17	Joback Method
cpg	854.98	J/mol×K	1095.21	Joback Method
cpg	862.41	J/mol×K	1134.24	Joback Method
cpg	868.78	J/mol×K	1173.28	Joback Method
dvisc	0.0003142	Pa×s	597.16	Joback Method

dvisc	0.0001976	Pa×s	654.14	Joback Method
dvisc	0.0001339	Pa×s	711.13	Joback Method
dvisc	0.0000961	Pa×s	768.11	Joback Method
dvisc	0.0000722	Pa×s	825.09	Joback Method
dvisc	0.0000563	Pa×s	882.08	Joback Method
dvisc	0.0000452	Pa×s	939.06	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=U378023&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