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

Inchi: InChI=1S/C24H29BrO4/c1-2-3-4-5-6-9-16-28-23(26)21-13-7-8-14-22(21)24(27)29-17-15-
InchiKey: YMIPCQXHDQHUCX-UHFFFAOYSA-N
Formula: C24H29BrO4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]: 461.39

Physical Properties

Property code	Value	Unit	Source
gf	-96.76	kJ/mol	Joback Method
hf	-551.84	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	6.366		Crippen Method
mcvol	333.880	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook
tb	1030.58	K	Joback Method
tc	1266.01	K	Joback Method
tf	642.24	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.20	J/mol×K	1030.58	Joback Method
cpg	1098.82	J/mol×K	1226.77	Joback Method
cpg	1091.33	J/mol×K	1187.53	Joback Method
cpg	1082.69	J/mol×K	1148.29	Joback Method
cpg	1072.83	J/mol×K	1109.06	Joback Method
cpg	1061.69	J/mol×K	1069.82	Joback Method
cpg	1105.23	J/mol×K	1266.01	Joback Method
dvisc	0.0000248	Pa×s	1030.58	Joback Method

dvisc	0.0000312	Pa×s	965.86	Joback Method
dvisc	0.0000407	Pa×s	901.13	Joback Method
dvisc	0.0000552	Pa×s	836.41	Joback Method
dvisc	0.0000789	Pa×s	771.69	Joback Method
dvisc	0.0001203	Pa×s	706.96	Joback Method
dvisc	0.0001996	Pa×s	642.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378027&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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