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

Inchi: InChI=1S/C21H23BrO4/c1-2-3-6-13-25-20(23)18-10-4-5-11-19(18)21(24)26-14-12-16-8-7

InchiKey: XDFLRRZGGXMGBK-UHFFFAOYSA-N

Formula: C21H23BrO4

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

Mol. weight [g/mol]: 419.31

Physical Properties

Property code	Value	Unit	Source
gf	-122.02	kJ/mol	Joback Method
hf	-489.92	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	92.96	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.196		Crippen Method
mcvol	291.610	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2887.00		NIST Webbook
tb	961.94	K	Joback Method
tc	1195.16	K	Joback Method
tf	608.43	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.72	J/mol×K	961.94	Joback Method
cpg	883.96	J/mol×K	1000.81	Joback Method
cpg	894.93	J/mol×K	1039.68	Joback Method
cpg	904.68	J/mol×K	1078.55	Joback Method
cpg	913.26	J/mol×K	1117.42	Joback Method
cpg	920.74	J/mol×K	1156.29	Joback Method
cpg	927.15	J/mol×K	1195.16	Joback Method
dvisc	0.0002818	Pa×s	608.43	Joback Method
dvisc	0.0001753	Pa×s	667.35	Joback Method

dvisc	0.0001177	Pa×s	726.27	Joback Method
dvisc	0.0000839	Pa×s	785.18	Joback Method
dvisc	0.0000628	Pa×s	844.10	Joback Method
dvisc	0.0000487	Pa×s	903.02	Joback Method
dvisc	0.0000390	Pa×s	961.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378024&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