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

Inchi: InChI=1S/C22H25BrO4/c1-2-3-4-7-14-26-21(24)19-11-5-6-12-20(19)22(25)27-15-13-17-9

InchiKey: JLTCLWBMSQWPQS-UHFFFAOYSA-N

Formula: C22H25BrO4

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

Mol. weight [g/mol]: 433.34

Physical Properties

Property code	Value	Unit	Source
gf	-113.60	kJ/mol	Joback Method
hf	-510.56	kJ/mol	Joback Method
hfus	50.90	kJ/mol	Joback Method
hvap	95.19	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.586		Crippen Method
mcvol	305.700	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tb	984.82	K	Joback Method
tc	1217.88	K	Joback Method
tf	619.70	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.34	J/mol×K	984.82	Joback Method
cpg	979.60	J/mol×K	1179.04	Joback Method
cpg	972.10	J/mol×K	1140.19	Joback Method
cpg	963.48	J/mol×K	1101.35	Joback Method
cpg	953.69	J/mol×K	1062.51	Joback Method
cpg	942.66	J/mol×K	1023.66	Joback Method
cpg	986.02	J/mol×K	1217.88	Joback Method
dvisc	0.0000336	Pa×s	984.82	Joback Method

dvisc	0.0000421	Pa×s	923.97	Joback Method
dvisc	0.0000544	Pa×s	863.11	Joback Method
dvisc	0.0000732	Pa×s	802.26	Joback Method
dvisc	0.0001033	Pa×s	741.41	Joback Method
dvisc	0.0001550	Pa×s	680.55	Joback Method
dvisc	0.0002520	Pa×s	619.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378025&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

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