

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

Inchi:	InChI=1S/C19H19BrO4/c1-2-11-23-18(21)16-8-3-4-9-17(16)19(22)24-12-10-14-6-5-7-15
InchiKey:	AIXPXQBIGCFDQK-UHFFFAOYSA-N
Formula:	C19H19BrO4
SMILES:	CCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	391.26

Physical Properties

Property code	Value	Unit	Source
gf	-138.86	kJ/mol	Joback Method
hf	-448.64	kJ/mol	Joback Method
hfus	43.13	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.415		Crippen Method
mcvol	263.430	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2689.00		NIST Webbook
tb	916.18	K	Joback Method
tc	1152.18	K	Joback Method
tf	585.89	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.39	J/mol×K	916.18	Joback Method
cpg	804.63	J/mol×K	1112.85	Joback Method
cpg	797.27	J/mol×K	1073.52	Joback Method
cpg	788.81	J/mol×K	1034.18	Joback Method
cpg	779.21	J/mol×K	994.85	Joback Method
cpg	768.42	J/mol×K	955.51	Joback Method
cpg	810.93	J/mol×K	1152.18	Joback Method
dvisc	0.0000523	Pa×s	916.18	Joback Method
dvisc	0.0000649	Pa×s	861.13	Joback Method

dvisc	0.0000829	Pa×s	806.08	Joback Method
dvisc	0.0001097	Pa×s	751.03	Joback Method
dvisc	0.0001518	Pa×s	695.99	Joback Method
dvisc	0.0002222	Pa×s	640.94	Joback Method
dvisc	0.0003492	Pa×s	585.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378021&Units=SI

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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