

Phthalic acid, 2-(4-bromophenyl)ethyl propyl ester

Inchi:	InChI=1S/C19H19BrO4/c1-2-12-23-18(21)16-5-3-4-6-17(16)19(22)24-13-11-14-7-9-15(20)
InchiKey:	YSWLNYQQTGRURE-UHFFFAOYSA-N
Formula:	C19H19BrO4
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Br)cc1
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	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	916.18	K	Joback Method
tc	1152.18	K	Joback Method
tf	585.89	K	Joback Method
vc	0.994	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.39	J/molxK	916.18	Joback Method
cpg	768.42	J/molxK	955.51	Joback Method
cpg	779.21	J/molxK	994.85	Joback Method
cpg	788.81	J/molxK	1034.18	Joback Method
cpg	797.27	J/molxK	1073.52	Joback Method
cpg	804.63	J/molxK	1112.85	Joback Method
cpg	810.93	J/molxK	1152.18	Joback Method
dvisc	0.0003492	Paxs	585.89	Joback Method

dvisc	0.0002222	Paxs	640.94	Joback Method
dvisc	0.0001518	Paxs	695.99	Joback Method
dvisc	0.0001097	Paxs	751.03	Joback Method
dvisc	0.0000829	Paxs	806.08	Joback Method
dvisc	0.0000649	Paxs	861.13	Joback Method
dvisc	0.0000523	Paxs	916.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U378035&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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