

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

Inchi:	InChI=1S/C20H21BrO4/c1-14(2)13-25-20(23)18-6-4-3-5-17(18)19(22)24-12-11-15-7-9-10
InchiKey:	DNQRHWCSJXHLPS-UHFFFAOYSA-N
Formula:	C20H21BrO4
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	405.28

Physical Properties

Property code	Value	Unit	Source
gf	-132.88	kJ/mol	Joback Method
hf	-474.56	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.661		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	938.62	K	Joback Method
tc	1175.56	K	Joback Method
tf	582.16	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.22	J/molxK	938.62	Joback Method
cpg	826.45	J/molxK	978.11	Joback Method
cpg	837.38	J/molxK	1017.60	Joback Method
cpg	847.07	J/molxK	1057.09	Joback Method
cpg	855.56	J/molxK	1096.58	Joback Method
cpg	862.91	J/molxK	1136.07	Joback Method
cpg	869.16	J/molxK	1175.56	Joback Method
dvisc	0.0003364	Paxs	582.16	Joback Method

dvisc	0.0002017	Paxs	641.57	Joback Method
dvisc	0.0001318	Paxs	700.98	Joback Method
dvisc	0.0000921	Paxs	760.39	Joback Method
dvisc	0.0000678	Paxs	819.80	Joback Method
dvisc	0.0000520	Paxs	879.21	Joback Method
dvisc	0.0000412	Paxs	938.62	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=U378036&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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