

Isophthalic acid, 4-bromophenyl butyl ester

Inchi:	InChI=1S/C18H17BrO4/c1-2-3-11-22-17(20)13-5-4-6-14(12-13)18(21)23-16-9-7-15(19)8
InchiKey:	WFVLQKJRYBPAAQ-UHFFFAOYSA-N
Formula:	C18H17BrO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	377.23

Physical Properties

Property code	Value	Unit	Source
gf	-147.28	kJ/mol	Joback Method
hf	-428.00	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.625		Crippen Method
mcvol	249.340	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	893.30	K	Joback Method
tc	1131.83	K	Joback Method
tf	574.62	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.78	J/molxK	893.30	Joback Method
cpg	711.67	J/molxK	933.06	Joback Method
cpg	722.33	J/molxK	972.81	Joback Method
cpg	731.82	J/molxK	1012.57	Joback Method
cpg	740.17	J/molxK	1052.32	Joback Method
cpg	747.42	J/molxK	1092.08	Joback Method
cpg	753.62	J/molxK	1131.83	Joback Method
dvisc	0.0003867	Paxs	574.62	Joback Method

dvisc	0.0002489	Paxs	627.73	Joback Method
dvisc	0.0001716	Paxs	680.85	Joback Method
dvisc	0.0001249	Paxs	733.96	Joback Method
dvisc	0.0000949	Paxs	787.07	Joback Method
dvisc	0.0000746	Paxs	840.19	Joback Method
dvisc	0.0000604	Paxs	893.30	Joback Method

Sources

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=U344466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

Latest version available from:

<https://www.chemeo.com/cid/99-304-5/Isophthalic-acid-4-bromophenyl-butyl-ester.pdf>

Generated by Cheméo on 2024-04-27 10:25:46.095500669 +0000 UTC m=+16502795.016077987.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.