

Isophthalic acid, 4-bromophenyl isobutyl ester

Inchi:	InChI=1S/C18H17BrO4/c1-12(2)11-22-17(20)13-4-3-5-14(10-13)18(21)23-16-8-6-15(19)
InchiKey:	AXKXFYADOWXRFP-UHFFFAOYSA-N
Formula:	C18H17BrO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	377.23

Physical Properties

Property code	Value	Unit	Source
gf	-149.72	kJ/mol	Joback Method
hf	-433.28	kJ/mol	Joback Method
hfus	37.02	kJ/mol	Joback Method
hvap	85.90	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.481		Crippen Method
mcvol	249.340	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2745.00		NIST Webbook
tb	892.86	K	Joback Method
tc	1134.84	K	Joback Method
tf	559.62	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.34	J/molxK	892.86	Joback Method
cpg	748.14	J/molxK	1094.51	Joback Method
cpg	740.95	J/molxK	1054.18	Joback Method
cpg	732.61	J/molxK	1013.85	Joback Method
cpg	723.10	J/molxK	973.52	Joback Method
cpg	712.35	J/molxK	933.19	Joback Method
cpg	754.23	J/molxK	1134.84	Joback Method
dvisc	0.0000552	Paxs	892.86	Joback Method
dvisc	0.0000691	Paxs	837.32	Joback Method

dvisc	0.0000894	Paxs	781.78	Joback Method
dvisc	0.0001202	Paxs	726.24	Joback Method
dvisc	0.0001697	Paxs	670.70	Joback Method
dvisc	0.0002552	Paxs	615.16	Joback Method
dvisc	0.0004160	Paxs	559.62	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=U344465&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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