

Isophthalic acid, 4-bromophenyl hexyl ester

Inchi:	InChI=1S/C20H21BrO4/c1-2-3-4-5-13-24-19(22)15-7-6-8-16(14-15)20(23)25-18-11-9-17
InchiKey:	BYIPAQC PFULTSQ-UHFFFAOYSA-N
Formula:	C20H21BrO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	405.28

Physical Properties

Property code	Value	Unit	Source
gf	-130.44	kJ/mol	Joback Method
hf	-469.28	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.405		Crippen Method
mvol	277.520	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	939.06	K	Joback Method
tc	1173.28	K	Joback Method
tf	597.16	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.72	J/molxK	939.06	Joback Method
cpg	825.86	J/molxK	978.10	Joback Method
cpg	836.75	J/molxK	1017.13	Joback Method
cpg	846.44	J/molxK	1056.17	Joback Method
cpg	854.98	J/molxK	1095.21	Joback Method
cpg	862.41	J/molxK	1134.24	Joback Method
cpg	868.78	J/molxK	1173.28	Joback Method
dvisc	0.0003142	Paxs	597.16	Joback Method

dvisc	0.0001976	Paxs	654.14	Joback Method
dvisc	0.0001339	Paxs	711.13	Joback Method
dvisc	0.0000961	Paxs	768.11	Joback Method
dvisc	0.0000722	Paxs	825.09	Joback Method
dvisc	0.0000563	Paxs	882.08	Joback Method
dvisc	0.0000452	Paxs	939.06	Joback Method

Sources

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=U344469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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