

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

Inchi:	InChI=1S/C24H20Br2O4/c25-19-9-5-17(6-10-19)13-15-29-23(27)21-3-1-2-4-22(21)24(28)
InchiKey:	GAOFTFQHEUFNSE-UHFFFAOYSA-N
Formula:	C24H20Br2O4
SMILES:	O=C(OCCc1ccc(Br)cc1)c1ccccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	532.22

Physical Properties

Property code	Value	Unit	Source
gf	20.34	kJ/mol	Joback Method
hf	-300.45	kJ/mol	Joback Method
hfus	55.02	kJ/mol	Joback Method
hvap	109.01	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	6.011		Crippen Method
mvol	327.620	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	3626.00		NIST Webbook
rinpol	3626.00		NIST Webbook
tb	1128.40	K	Joback Method
tc	1394.25	K	Joback Method
tf	740.98	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.92	J/molxK	1128.40	Joback Method
cpg	989.45	J/molxK	1349.94	Joback Method
cpg	985.01	J/molxK	1305.63	Joback Method
cpg	979.75	J/molxK	1261.33	Joback Method
cpg	973.56	J/molxK	1217.02	Joback Method
cpg	966.32	J/molxK	1172.71	Joback Method
cpg	993.18	J/molxK	1394.25	Joback Method
dvisc	0.0000197	Paxs	1128.40	Joback Method

dvisc	0.0000242	Paxs	1063.83	Joback Method
dvisc	0.0000306	Paxs	999.26	Joback Method
dvisc	0.0000398	Paxs	934.69	Joback Method
dvisc	0.0000540	Paxs	870.12	Joback Method
dvisc	0.0000767	Paxs	805.55	Joback Method
dvisc	0.0001160	Paxs	740.98	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=U378047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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