

Phthalic acid, di(2-methylbenzyl) ester

Inchi:	InChI=1S/C24H22O4/c1-17-9-3-5-11-19(17)15-27-23(25)21-13-7-8-14-22(21)24(26)28-1
InchiKey:	UJXAWKBKTUXCAE-UHFFFAOYSA-N
Formula:	C24H22O4
SMILES:	<chem>Cc1ccccc1COC(=O)c1ccccc1C(=O)OCc1ccccc1C</chem>
Mol. weight [g/mol]:	374.43

Physical Properties

Property code	Value	Unit	Source
gf	-8.30	kJ/mol	Joback Method
hf	-353.11	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	96.14	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	5.017		Crippen Method
mvol	292.620	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2880.00		NIST Webbook
tb	996.08	K	Joback Method
tc	1242.38	K	Joback Method
tf	621.38	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.66	J/molxK	996.08	Joback Method
cpg	918.43	J/molxK	1037.13	Joback Method
cpg	928.67	J/molxK	1078.18	Joback Method
cpg	937.44	J/molxK	1119.23	Joback Method
cpg	944.82	J/molxK	1160.28	Joback Method
cpg	950.85	J/molxK	1201.33	Joback Method
cpg	955.60	J/molxK	1242.38	Joback Method
dvisc	0.0002483	Paxs	621.38	Joback Method
dvisc	0.0001539	Paxs	683.83	Joback Method

dvisc	0.0001034	Paxs	746.28	Joback Method
dvisc	0.0000738	Paxs	808.73	Joback Method
dvisc	0.0000553	Paxs	871.18	Joback Method
dvisc	0.0000431	Paxs	933.63	Joback Method
dvisc	0.0000346	Paxs	996.08	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=U382863&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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