

Phthalic acid, 2-methylbenzyl nonyl ester

Inchi:	InChI=1S/C25H32O4/c1-3-4-5-6-7-8-13-18-28-24(26)22-16-11-12-17-23(22)25(27)29-19
InchiKey:	IYAJXIOTPDVLHK-UHFFFAOYSA-N
Formula:	C25H32O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C
Mol. weight [g/mol]:	396.52

Physical Properties

Property code	Value	Unit	Source
gf	-102.66	kJ/mol	Joback Method
hf	-598.81	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	95.43	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.259		Crippen Method
mvol	330.470	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2862.00		NIST Webbook
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tb	987.30	K	Joback Method
tc	1212.72	K	Joback Method
tf	593.71	K	Joback Method
vc	1.268	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.99	J/molxK	987.30	Joback Method
cpg	1090.36	J/molxK	1024.87	Joback Method
cpg	1103.28	J/molxK	1062.44	Joback Method
cpg	1114.80	J/molxK	1100.01	Joback Method
cpg	1124.97	J/molxK	1137.58	Joback Method
cpg	1133.85	J/molxK	1175.15	Joback Method
cpg	1141.48	J/molxK	1212.72	Joback Method
dvisc	0.0002692	Paxs	593.71	Joback Method

dvisc	0.0001532	Paxs	659.31	Joback Method
dvisc	0.0000965	Paxs	724.91	Joback Method
dvisc	0.0000657	Paxs	790.50	Joback Method
dvisc	0.0000474	Paxs	856.10	Joback Method
dvisc	0.0000358	Paxs	921.70	Joback Method
dvisc	0.0000281	Paxs	987.30	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=U382855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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