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
mcvol	330.470	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	987.30	K	Joback Method
tc	1212.72	K	Joback Method
tf	593.71	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.99	J/mol×K	987.30	Joback Method
cpg	1133.85	J/mol×K	1175.15	Joback Method
cpg	1124.97	J/mol×K	1137.58	Joback Method
cpg	1114.80	J/mol×K	1100.01	Joback Method
cpg	1103.28	J/mol×K	1062.44	Joback Method
cpg	1090.36	J/mol×K	1024.87	Joback Method
cpg	1141.48	J/mol×K	1212.72	Joback Method
dvisc	0.0000281	Pa×s	987.30	Joback Method

dvisc	0.0000358	Pa×s	921.70	Joback Method
dvisc	0.0000474	Pa×s	856.10	Joback Method
dvisc	0.0000657	Pa×s	790.50	Joback Method
dvisc	0.0000965	Pa×s	724.91	Joback Method
dvisc	0.0001532	Pa×s	659.31	Joback Method
dvisc	0.0002692	Pa×s	593.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382855&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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