Phthalic acid, methyl nonyl ester

Other names: 1,2-Benzenedicarboxylic acid, nonyl methyl ester
Inchi: InChI=1S/C18H26O4/c1-3-4-5-6-7-8-11-14-22-18(20)16-13-10-9-12-15(16)17(19)21-2/h9
InchiKey: FCOLFBWVCBQMTQ-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
af	0.9304		Cheméo Relay (1.0)
hf	-765.60	kJ/mol	Cheméo Relay (1.0)
hfus	41.60	kJ/mol	Joback Method
hvap	94.58	kJ/mol	Cheméo Relay (1.0)
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-5.41		Cheméo Relay (1.0)
logp	4.381		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	613.59	K	Cheméo Relay (1.0)
tc	820.54	K	Cheméo Relay (1.0)
tf	272.14	K	Cheméo Relay (1.0)
vc	0.963	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.25	J/mol×K	795.48	Joback Method
cpg	839.97	J/mol×K	995.15	Joback Method
cpg	829.35	J/mol×K	961.87	Joback Method
cpg	817.75	J/mol×K	928.59	Joback Method
cpg	805.16	J/mol×K	895.32	Joback Method
cpg	791.55	J/mol×K	862.04	Joback Method

cpg	776.92	J/mol×K	828.76	Joback Method
dvisc	0.0001703	Pa×s	635.68	Joback Method
dvisc	0.0000720	Pa×s	795.48	Joback Method
dvisc	0.0000921	Pa×s	742.21	Joback Method
dvisc	0.0001223	Pa×s	688.95	Joback Method
dvisc	0.0007181	Pa×s	475.88	Joback Method
dvisc	0.0002520	Pa×s	582.41	Joback Method
dvisc	0.0004036	Pa×s	529.15	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91485824&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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