Phthalic acid, 3,3-dimethylbut-2-yl nonyl ester

Inchi: InChI=1S/C23H36O4/c1-6-7-8-9-10-11-14-17-26-21(24)19-15-12-13-16-20(19)22(25)27-
InchiKey: GBAWGQNEEOBINP-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-221.88	kJ/mol	Joback Method
hf	-796.62	kJ/mol	Joback Method
hfus	43.62	kJ/mol	Joback Method
hvap	86.36	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.185		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2526.00		NIST Webbook
tb	906.21	K	Joback Method
tc	1115.53	K	Joback Method
tf	519.65	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.87	J/mol×K	906.21	Joback Method
cpg	1075.76	J/mol×K	941.10	Joback Method
cpg	1091.37	J/mol×K	975.98	Joback Method
cpg	1105.75	J/mol×K	1010.87	Joback Method
cpg	1118.97	J/mol×K	1045.76	Joback Method
cpg	1131.08	J/mol×K	1080.64	Joback Method
cpg	1142.12	J/mol×K	1115.53	Joback Method
dvisc	0.0004367	Pa×s	519.65	Joback Method
dvisc	0.0002089	Pa×s	584.08	Joback Method

dvisc	0.0001157	Pa×s	648.50	Joback Method
dvisc	0.0000713	Pa×s	712.93	Joback Method
dvisc	0.0000476	Pa×s	777.36	Joback Method
dvisc	0.0000338	Pa×s	841.78	Joback Method
dvisc	0.0000252	Pa×s	906.21	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=U357008&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