Methyl 3,5,5-trimethylhexyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 3,5,5-trimethylhexyl methyl ester
Inchi: InChI=1S/C18H26O4/c1-13(12-18(2,3)4)10-11-22-17(20)15-9-7-6-8-14(15)16(19)21-5/h6
InchiKey: SHDCJNQVKUNGAG-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: COC(=O)c1ccccc1C(=O)OCCC(C)CC(C)(C)C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-263.98	kJ/mol	Joback Method
hf	-693.42	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.092		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2101.00		NIST Webbook
tb	791.81	K	Joback Method
tc	1001.25	K	Joback Method
tf	463.30	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.36	J/mol×K	791.81	Joback Method
cpg	833.02	J/mol×K	966.34	Joback Method
cpg	821.22	J/mol×K	931.44	Joback Method
cpg	808.40	J/mol×K	896.53	Joback Method
cpg	794.50	J/mol×K	861.62	Joback Method
cpg	779.50	J/mol×K	826.72	Joback Method
cpg	843.81	J/mol×K	1001.25	Joback Method
dvisc	0.0000533	Pa×s	791.81	Joback Method

dvisc	0.0000707	Pa×s	737.06	Joback Method
dvisc	0.0000980	Pa×s	682.31	Joback Method
dvisc	0.0001438	Pa×s	627.55	Joback Method
dvisc	0.0002272	Pa×s	572.80	Joback Method
dvisc	0.0003954	Pa×s	518.05	Joback Method
dvisc	0.0007844	Pa×s	463.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373814&Units=SI
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

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