Phthalic acid, 2,4-dimethylpent-3-yl octyl ester

Inchi: InChI=1S/C23H36O4/c1-6-7-8-9-10-13-16-26-22(24)19-14-11-12-15-20(19)23(25)27-21(
InchiKey: ZHSIFOJHDSSTCO-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-229.60	kJ/mol	Joback Method
hf	-798.43	kJ/mol	Joback Method
hfus	43.98	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.041		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2495.00		NIST Webbook
tb	908.56	K	Joback Method
tc	1117.17	K	Joback Method
tf	487.23	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.44	J/mol×K	908.56	Joback Method
cpg	1076.35	J/mol×K	943.33	Joback Method
cpg	1091.90	J/mol×K	978.10	Joback Method
cpg	1106.12	J/mol×K	1012.87	Joback Method
cpg	1119.04	J/mol×K	1047.64	Joback Method
cpg	1130.71	J/mol×K	1082.41	Joback Method
cpg	1141.15	J/mol×K	1117.17	Joback Method
dvisc	0.0006337	Pa×s	487.23	Joback Method
dvisc	0.0002694	Pa×s	557.45	Joback Method

dvisc	0.0001387	Pa×s	627.67	Joback Method
dvisc	0.0000816	Pa×s	697.89	Joback Method
dvisc	0.0000529	Pa×s	768.12	Joback Method
dvisc	0.0000369	Pa×s	838.34	Joback Method
dvisc	0.0000272	Pa×s	908.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356847&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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