Phthalic acid, 2,3-dimethylphenyl octyl ester

Inchi: InChI=1S/C24H30O4/c1-4-5-6-7-8-11-17-27-23(25)20-14-9-10-15-21(20)24(26)28-22-16
InchiKey: LKZUBSVJXTZQNY-UHFFFAOYSA-N
Formula: C24H30O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 382.49

Physical Properties

Property code	Value	Unit	Source
gf	-120.71	kJ/mol	Joback Method
hf	-589.64	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.040		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2861.00		NIST Webbook
tb	969.40	K	Joback Method
tc	1193.86	K	Joback Method
tf	594.96	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.67	J/mol×K	969.40	Joback Method
cpg	1028.85	J/mol×K	1006.81	Joback Method
cpg	1041.60	J/mol×K	1044.22	Joback Method
cpg	1052.96	J/mol×K	1081.63	Joback Method
cpg	1062.96	J/mol×K	1119.04	Joback Method
cpg	1071.65	J/mol×K	1156.45	Joback Method
cpg	1079.05	J/mol×K	1193.86	Joback Method
dvisc	0.0002694	Pa×s	594.96	Joback Method
dvisc	0.0001612	Pa×s	657.37	Joback Method

dvisc	0.0001054	Pa×s	719.77	Joback Method
dvisc	0.0000738	Pa×s	782.18	Joback Method
dvisc	0.0000544	Pa×s	844.59	Joback Method
dvisc	0.0000419	Pa×s	906.99	Joback Method
dvisc	0.0000333	Pa×s	969.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357090&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