Isophthalic acid, 3,7-dimethyloct-6-enyl hexyl ester

Inchi: InChI=1S/C24H36O4/c1-5-6-7-8-16-27-23(25)21-13-10-14-22(18-21)24(26)28-17-15-20(

InchiKey: FJSLZXKXWNBHHY-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-144.63	kJ/mol	Joback Method
hf	-701.08	kJ/mol	Joback Method
hfus	52.51	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.353		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2776.00		NIST Webbook
tb	936.36	K	Joback Method
tc	1149.09	K	Joback Method
tf	509.46	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.58	J/mol×K	936.36	Joback Method
cpg	1108.29	J/mol×K	971.82	Joback Method
cpg	1123.73	J/mol×K	1007.27	Joback Method
cpg	1137.96	J/mol×K	1042.73	Joback Method
cpg	1151.03	J/mol×K	1078.18	Joback Method
cpg	1162.98	J/mol×K	1113.64	Joback Method
cpg	1173.87	J/mol×K	1149.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356740&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
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