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

Inchi: InChI=1S/C26H40O4/c1-5-6-7-8-9-10-18-29-25(27)23-15-12-16-24(20-23)26(28)30-19-1

InchiKey: WULLPAYPKOUGQS-UHFFFAOYSA-N

Formula: C26H40O4

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

Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-127.79	kJ/mol	Joback Method
hf	-742.36	kJ/mol	Joback Method
hfus	57.69	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.133		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	982.12	K	Joback Method
tc	1202.45	K	Joback Method
tf	532.00	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.30	J/mol×K	982.12	Joback Method
cpg	1232.50	J/mol×K	1018.84	Joback Method
cpg	1248.33	J/mol×K	1055.56	Joback Method
cpg	1262.83	J/mol×K	1092.28	Joback Method
cpg	1276.09	J/mol×K	1129.00	Joback Method
cpg	1288.16	J/mol×K	1165.73	Joback Method
cpg	1299.10	J/mol×K	1202.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356742&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