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

Inchi: InChI=1S/C28H44O4/c1-5-6-7-8-9-10-11-12-20-31-27(29)25-17-14-18-26(22-25)28(30)3
InchiKey: ADNSUFQCXIRRBA-UHFFFAOYSA-N
Formula: C28H44O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1
Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-110.95	kJ/mol	Joback Method
hf	-783.64	kJ/mol	Joback Method
hfus	62.87	kJ/mol	Joback Method
hvap	98.82	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.913		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	848.50	kPa	Joback Method
rinpol	3192.00		NIST Webbook
tb	1027.88	K	Joback Method
tc	1259.95	K	Joback Method
tf	554.54	K	Joback Method
vc	1.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.90	J/mol×K	1027.88	Joback Method
cpg	1358.75	J/mol×K	1066.56	Joback Method
cpg	1375.05	J/mol×K	1105.24	Joback Method
cpg	1389.91	J/mol×K	1143.92	Joback Method
cpg	1403.40	J/mol×K	1182.60	Joback Method
cpg	1415.60	J/mol×K	1221.27	Joback Method
cpg	1426.60	J/mol×K	1259.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356743&Units=SI

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

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