Isophthalic acid, hexadecyl 2-methylprop-2-en-1-yl ester

Inchi: InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-31-27(29)25-19-18-20

InchiKey: SVVYYRPJZBKZGE-UHFFFAOYSA-N

Formula: C28H44O4

SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCCC)c1

Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-100.89	kJ/mol	Joback Method
hf	-770.15	kJ/mol	Joback Method
hfus	64.91	kJ/mol	Joback Method
hvap	98.58	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	3341.00		NIST Webbook
rinpol	3341.00		NIST Webbook
tb	1020.84	K	Joback Method
tc	1252.51	K	Joback Method
tf	572.86	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.87	J/mol×K	1020.84	Joback Method
cpg	1356.65	J/mol×K	1059.45	Joback Method
cpg	1372.80	J/mol×K	1098.06	Joback Method
cpg	1387.38	J/mol×K	1136.68	Joback Method
cpg	1400.48	J/mol×K	1175.29	Joback Method
cpg	1412.16	J/mol×K	1213.90	Joback Method
cpg	1422.50	J/mol×K	1252.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343957&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

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