Phthalic acid, 3-methylbut-3-enyl octadecyl ester

Inchi: InChI=1S/C31H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-34-30(32)28-22

InchiKey: NPMDQVAMWAWDEM-UHFFFAOYSA-N

Formula: C31H50O4

SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 486.73

Physical Properties

Property code	Value	Unit	Source
gf	-75.63	kJ/mol	Joback Method
hf	-832.07	kJ/mol	Joback Method
hfus	72.68	kJ/mol	Joback Method
hvap	105.26	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	9.228		Crippen Method
mcvol	434.470	ml/mol	McGowan Method
pc	715.30	kPa	Joback Method
rinpol	3452.00		NIST Webbook
tb	1089.48	K	Joback Method
tc	1349.96	K	Joback Method
tf	606.67	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1529.58	J/mol×K	1089.48	Joback Method
cpg	1548.62	J/mol×K	1132.89	Joback Method
cpg	1565.61	J/mol×K	1176.31	Joback Method
cpg	1580.68	J/mol×K	1219.72	Joback Method
cpg	1593.95	J/mol×K	1263.13	Joback Method
cpg	1605.53	J/mol×K	1306.55	Joback Method
cpg	1615.56	J/mol×K	1349.96	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=U360269&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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