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

Inchi: InChI=1S/C30H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-33-29(31)27-21-18
InchiKey: FVTSQWTVWBIJMT-UHFFFAOYSA-N
Formula: C30H48O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-84.05	kJ/mol	Joback Method
hf	-811.43	kJ/mol	Joback Method
hfus	70.09	kJ/mol	Joback Method
hvap	103.03	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.838		Crippen Method
mcvol	420.380	ml/mol	McGowan Method
pc	753.50	kPa	Joback Method
rinpol	3348.00		NIST Webbook
rinpol	3348.00		NIST Webbook
tb	1066.60	K	Joback Method
tc	1316.10	K	Joback Method
tf	595.40	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.70	J/mol×K	1066.60	Joback Method
cpg	1484.28	J/mol×K	1108.18	Joback Method
cpg	1500.97	J/mol×K	1149.77	Joback Method
cpg	1515.87	J/mol×K	1191.35	Joback Method
cpg	1529.08	J/mol×K	1232.94	Joback Method
cpg	1540.70	J/mol×K	1274.52	Joback Method
cpg	1550.85	J/mol×K	1316.10	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=U360265&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