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

Inchi: InChI=1S/C29H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-23-32-28(30)26-20-17-18

InchiKey: YBEFGDQROIWZRM-UHFFFAOYSA-N

Formula: C29H46O4

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

Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-92.47	kJ/mol	Joback Method
hf	-790.79	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mcvol	406.290	ml/mol	McGowan Method
pc	794.84	kPa	Joback Method
rinpol	3246.00		NIST Webbook
tb	1043.72	K	Joback Method
tc	1283.65	K	Joback Method
tf	584.13	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.12	J/mol×K	1043.72	Joback Method
cpg	1420.28	J/mol×K	1083.71	Joback Method
cpg	1436.69	J/mol×K	1123.70	Joback Method
cpg	1451.42	J/mol×K	1163.69	Joback Method
cpg	1464.58	J/mol×K	1203.68	Joback Method
cpg	1476.24	J/mol×K	1243.66	Joback Method
cpg	1486.49	J/mol×K	1283.65	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=U357114&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