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

Inchi: InChI=1S/C26H40O4/c1-4-5-6-7-8-9-10-11-12-13-16-20-29-25(27)23-17-14-15-18-24(23
InchiKey: ZSPYOCZBRXMJER-UHFFFAOYSA-N
Formula: C26H40O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-117.73	kJ/mol	Joback Method
hf	-728.87	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2939.00		NIST Webbook
tb	975.08	K	Joback Method
tc	1193.80	K	Joback Method
tf	550.32	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.51	J/mol×K	975.08	Joback Method
cpg	1230.65	J/mol×K	1011.53	Joback Method
cpg	1246.35	J/mol×K	1047.99	Joback Method
cpg	1260.66	J/mol×K	1084.44	Joback Method
cpg	1273.63	J/mol×K	1120.89	Joback Method
cpg	1285.33	J/mol×K	1157.35	Joback Method
cpg	1295.81	J/mol×K	1193.80	Joback Method

Sources

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=U357111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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