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

Inchi: InChI=1S/C24H36O4/c1-4-5-6-7-8-9-10-11-14-18-27-23(25)21-15-12-13-16-22(21)24(26

InchiKey: AYJKJJRCSIHIOD-UHFFFAOYSA-N

Formula: C24H36O4

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

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-134.57	kJ/mol	Joback Method
hf	-687.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2733.00		NIST Webbook
tb	929.32	K	Joback Method
tc	1139.31	K	Joback Method
tf	527.78	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.97	J/mol×K	929.32	Joback Method
cpg	1106.59	J/mol×K	964.32	Joback Method
cpg	1121.92	J/mol×K	999.32	Joback Method
cpg	1135.98	J/mol×K	1034.32	Joback Method
cpg	1148.84	J/mol×K	1069.32	Joback Method
cpg	1160.52	J/mol×K	1104.31	Joback Method
cpg	1171.08	J/mol×K	1139.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357109&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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