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

Inchi: InChI=1S/C25H38O4/c1-4-5-6-7-8-9-10-11-12-15-19-28-24(26)22-16-13-14-17-23(22)25

InchiKey: RJMGQWPKENWAPJ-UHFFFAOYSA-N

Formula: C25H38O4

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

Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-126.15	kJ/mol	Joback Method
hf	-708.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	91.90	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.887		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2835.00		NIST Webbook
tb	952.20	K	Joback Method
tc	1166.06	K	Joback Method
tf	539.05	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.49	J/mol×K	952.20	Joback Method
cpg	1168.35	J/mol×K	987.84	Joback Method
cpg	1183.86	J/mol×K	1023.49	Joback Method
cpg	1198.04	J/mol×K	1059.13	Joback Method
cpg	1210.96	J/mol×K	1094.78	Joback Method
cpg	1222.66	J/mol×K	1130.42	Joback Method
cpg	1233.18	J/mol×K	1166.06	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=U357110&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