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

Inchi: InChI=1S/C21H30O4/c1-4-5-6-7-8-11-15-24-20(22)18-12-9-10-13-19(18)21(23)25-16-14
InchiKey: SLMOCUOIZQZIOV-UHFFFAOYSA-N
Formula: C21H30O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-159.83	kJ/mol	Joback Method
hf	-625.67	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	2435.00		NIST Webbook
tb	860.68	K	Joback Method
tc	1064.32	K	Joback Method
tf	493.97	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.00	J/mol×K	860.68	Joback Method
cpg	924.98	J/mol×K	894.62	Joback Method
cpg	939.81	J/mol×K	928.56	Joback Method
cpg	953.53	J/mol×K	962.50	Joback Method
cpg	966.16	J/mol×K	996.44	Joback Method
cpg	977.74	J/mol×K	1030.38	Joback Method
cpg	988.30	J/mol×K	1064.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357106&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