Isophthalic acid, 3-methylbut-2-en-1-yl octyl ester

Inchi: InChI=1S/C21H30O4/c1-4-5-6-7-8-9-14-24-20(22)18-11-10-12-19(16-18)21(23)25-15-13

InchiKey: ZEYYHAOHFREYFN-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-167.45	kJ/mol	Joback Method
hf	-633.88	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	83.63	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	868.16	K	Joback Method
tc	1074.35	K	Joback Method
tf	490.65	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.91	J/mol×K	868.16	Joback Method
cpg	925.91	J/mol×K	902.52	Joback Method
cpg	940.80	J/mol×K	936.89	Joback Method
cpg	954.61	J/mol×K	971.25	Joback Method
cpg	967.38	J/mol×K	1005.62	Joback Method
cpg	979.14	J/mol×K	1039.98	Joback Method
cpg	989.94	J/mol×K	1074.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343940&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

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