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

Inchi: InChI=1S/C20H28O4/c1-4-5-6-7-8-13-23-19(21)17-10-9-11-18(15-17)20(22)24-14-12-16

InchiKey: OIRUZSBCEFAKEE-UHFFFAOYSA-N

Formula: C20H28O4

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

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-175.87	kJ/mol	Joback Method
hf	-613.24	kJ/mol	Joback Method
hfus	45.67	kJ/mol	Joback Method
hvap	81.40	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		NIST Webbook
tb	845.28	K	Joback Method
tc	1051.09	K	Joback Method
tf	479.38	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.90	J/mol×K	845.28	Joback Method
cpg	866.69	J/mol×K	879.58	Joback Method
cpg	881.40	J/mol×K	913.88	Joback Method
cpg	895.05	J/mol×K	948.18	Joback Method
cpg	907.69	J/mol×K	982.49	Joback Method
cpg	919.35	J/mol×K	1016.79	Joback Method
cpg	930.07	J/mol×K	1051.09	Joback Method

Sources

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=U343939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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