Isophthalic acid, heptyl 2-methylprop-2-en-1-yl ester

Inchi: InChI=1S/C19H26O4/c1-4-5-6-7-8-12-22-18(20)16-10-9-11-17(13-16)19(21)23-14-15(2)3

InchiKey: FTNXBVVWFDNDKJ-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCCCCCC)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-176.67	kJ/mol	Joback Method
hf	-584.39	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.547		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2394.00		NIST Webbook
tb	814.92	K	Joback Method
tc	1018.11	K	Joback Method
tf	471.43	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.95	J/mol×K	814.92	Joback Method
cpg	807.51	J/mol×K	848.79	Joback Method
cpg	821.99	J/mol×K	882.65	Joback Method
cpg	835.43	J/mol×K	916.52	Joback Method
cpg	847.85	J/mol×K	950.38	Joback Method
cpg	859.27	J/mol×K	984.25	Joback Method
cpg	869.72	J/mol×K	1018.11	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=U343950&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