Isophthalic acid, isohexyl 2-methylbutyl ester

Inchi: InChI=1S/C19H28O4/c1-5-15(4)13-23-19(21)17-10-6-9-16(12-17)18(20)22-11-7-8-14(2)3
InchiKey: BPRICPALKQFPBV-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCC(C)COC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-260.84	kJ/mol	Joback Method
hf	-710.59	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.482		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	817.48	K	Joback Method
tc	1021.25	K	Joback Method
tf	457.15	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.12	J/mol×K	817.48	Joback Method
cpg	836.35	J/mol×K	851.44	Joback Method
cpg	851.44	J/mol×K	885.40	Joback Method
cpg	865.39	J/mol×K	919.36	Joback Method
cpg	878.23	J/mol×K	953.32	Joback Method
cpg	889.98	J/mol×K	987.28	Joback Method
cpg	900.66	J/mol×K	1021.25	Joback Method
dvisc	0.0008629	Pa×s	457.15	Joback Method
dvisc	0.0004138	Pa×s	517.21	Joback Method

dvisc	0.0002312	Pa×s	577.26	Joback Method
dvisc	0.0001441	Pa×s	637.32	Joback Method
dvisc	0.0000975	Pa×s	697.37	Joback Method
dvisc	0.0000702	Pa×s	757.42	Joback Method
dvisc	0.0000530	Pa×s	817.48	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=U344732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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