Isophthalic acid, dec-2-yl isohexyl ester

Inchi: InChI=1S/C24H38O4/c1-5-6-7-8-9-10-14-20(4)28-24(26)22-16-11-15-21(18-22)23(25)27
InchiKey: VVKRIXRQRGGBSC-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCCCC(C)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-218.74	kJ/mol	Joback Method
hf	-813.79	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.575		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2693.00		NIST Webbook
tb	931.88	K	Joback Method
tc	1142.43	K	Joback Method
tf	513.50	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.29	J/mol×K	931.88	Joback Method
cpg	1137.32	J/mol×K	966.97	Joback Method
cpg	1152.94	J/mol×K	1002.06	Joback Method
cpg	1167.20	J/mol×K	1037.16	Joback Method
cpg	1180.14	J/mol×K	1072.25	Joback Method
cpg	1191.79	J/mol×K	1107.34	Joback Method
cpg	1202.19	J/mol×K	1142.43	Joback Method
dvisc	0.0004856	Pa×s	513.50	Joback Method
dvisc	0.0002219	Pa×s	583.23	Joback Method

dvisc	0.0001198	Pa×s	652.96	Joback Method
dvisc	0.0000729	Pa×s	722.69	Joback Method
dvisc	0.0000484	Pa×s	792.42	Joback Method
dvisc	0.0000343	Pa×s	862.15	Joback Method
dvisc	0.0000256	Pa×s	931.88	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=U356513&Units=SI

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

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