Isophthalic acid, phenylethyl undecyl ester

Inchi: InChI=1S/C27H36O4/c1-2-3-4-5-6-7-8-9-13-20-30-26(28)24-17-14-18-25(22-24)27(29)31
InchiKey: MZTHESWYWUYZLZ-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-76.19	kJ/mol	Joback Method
hf	-628.62	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.774		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	3416.00		NIST Webbook
rinpol	3416.00		NIST Webbook
tb	1028.08	K	Joback Method
tc	1259.02	K	Joback Method
tf	603.73	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.95	J/mol×K	1028.08	Joback Method
cpg	1257.89	J/mol×K	1220.53	Joback Method
cpg	1248.86	J/mol×K	1182.04	Joback Method
cpg	1238.53	J/mol×K	1143.55	Joback Method
cpg	1226.81	J/mol×K	1105.06	Joback Method
cpg	1213.64	J/mol×K	1066.57	Joback Method
cpg	1265.69	J/mol×K	1259.02	Joback Method
dvisc	0.0000203	Pa×s	1028.08	Joback Method

dvisc	0.0000263	Pa×s	957.35	Joback Method
dvisc	0.0000355	Pa×s	886.63	Joback Method
dvisc	0.0000505	Pa×s	815.90	Joback Method
dvisc	0.0000768	Pa×s	745.18	Joback Method
dvisc	0.0001276	Pa×s	674.46	Joback Method
dvisc	0.0002386	Pa×s	603.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344341&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
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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