Isophthalic acid, hexyl phenylethyl ester

Inchi: InChI=1S/C22H26O4/c1-2-3-4-8-15-25-21(23)19-12-9-13-20(17-19)22(24)26-16-14-18-1
InchiKey: DMVVRTCCGIAJCT-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-118.29	kJ/mol	Joback Method
hf	-525.42	kJ/mol	Joback Method
hfus	46.00	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.823		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2880.00		NIST Webbook
tb	913.68	K	Joback Method
tc	1135.36	K	Joback Method
tf	547.38	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.84	J/mol×K	913.68	Joback Method
cpg	956.76	J/mol×K	1098.41	Joback Method
cpg	947.44	J/mol×K	1061.47	Joback Method
cpg	936.93	J/mol×K	1024.52	Joback Method
cpg	925.19	J/mol×K	987.57	Joback Method
cpg	912.17	J/mol×K	950.63	Joback Method
cpg	964.94	J/mol×K	1135.36	Joback Method
dvisc	0.0000424	Pa×s	913.68	Joback Method
dvisc	0.0000543	Pa×s	852.63	Joback Method

dvisc	0.0000721	Pa×s	791.58	Joback Method
dvisc	0.0001003	Pa×s	730.53	Joback Method
dvisc	0.0001483	Pa×s	669.48	Joback Method
dvisc	0.0002373	Pa×s	608.43	Joback Method
dvisc	0.0004215	Pa×s	547.38	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=U344337&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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