Isophthalic acid, 2-cyclohexylethyl isobutyl ester

Inchi: InChI=1S/C20H28O4/c1-15(2)14-24-20(22)18-10-6-9-17(13-18)19(21)23-12-11-16-7-4-3

InchiKey: ASITXOKUHAKVLW-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: CC(C)COC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-225.53	kJ/mol	Joback Method
hf	-671.63	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.627		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	860.35	K	Joback Method
tc	1082.33	K	Joback Method
tf	490.80	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.42	J/mol×K	860.35	Joback Method
cpg	944.18	J/mol×K	1045.34	Joback Method
cpg	932.96	J/mol×K	1008.34	Joback Method
cpg	920.31	J/mol×K	971.34	Joback Method
cpg	906.19	J/mol×K	934.34	Joback Method
cpg	890.57	J/mol×K	897.35	Joback Method
cpg	953.99	J/mol×K	1082.33	Joback Method
dvisc	0.0000520	Pa×s	860.35	Joback Method

dvisc	0.0000684	Pa×s	798.76	Joback Method
dvisc	0.0000944	Pa×s	737.17	Joback Method
dvisc	0.0001381	Pa×s	675.57	Joback Method
dvisc	0.0002180	Pa×s	613.98	Joback Method
dvisc	0.0003810	Pa×s	552.39	Joback Method
dvisc	0.0007660	Pa×s	490.80	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=U343810&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