Isophthalic acid, 2-cyclohexylethyl ethyl ester

Inchi: InChI=1S/C18H24O4/c1-2-21-17(19)15-9-6-10-16(13-15)18(20)22-12-11-14-7-4-3-5-8-14
InchiKey: KJWCULJNELDRMZ-UHFFFAOYSA-N
Formula: C18H24O4
SMILES: CCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-239.93	kJ/mol	Joback Method
hf	-625.07	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.990		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2429.00		NIST Webbook
rinpol	2429.00		NIST Webbook
tb	815.03	K	Joback Method
tc	1038.33	K	Joback Method
tf	483.26	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.87	J/mol×K	815.03	Joback Method
cpg	826.83	J/mol×K	1001.11	Joback Method
cpg	815.43	J/mol×K	963.90	Joback Method
cpg	802.66	J/mol×K	926.68	Joback Method
cpg	788.49	J/mol×K	889.46	Joback Method
cpg	772.90	J/mol×K	852.25	Joback Method
cpg	836.90	J/mol×K	1038.33	Joback Method
dvisc	0.0000749	Pa×s	815.03	Joback Method

dvisc	0.0000965	Pa×s	759.73	Joback Method
dvisc	0.0001296	Pa×s	704.44	Joback Method
dvisc	0.0001828	Pa×s	649.14	Joback Method
dvisc	0.0002751	Pa×s	593.85	Joback Method
dvisc	0.0004502	Pa×s	538.55	Joback Method
dvisc	0.0008245	Pa×s	483.26	Joback Method

Sources

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=U343808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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