Isophthalic acid, ethyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C17H22O4/c1-3-20-16(18)13-8-6-9-14(11-13)17(19)21-15-10-5-4-7-12(15)2/h6

InchiKey: KXZMUFYBAJVJCQ-UHFFFAOYSA-N

Formula: C17H22O4

SMILES: CCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-256.06	kJ/mol	Joback Method
hf	-624.77	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.599		Crippen Method
mcvol	230.650	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook
tb	787.48	K	Joback Method
tc	1013.74	K	Joback Method
tf	467.75	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.00	J/mol×K	787.48	Joback Method
cpg	719.50	J/mol×K	825.19	Joback Method
cpg	735.53	J/mol×K	862.90	Joback Method
cpg	750.09	J/mol×K	900.61	Joback Method
cpg	763.21	J/mol×K	938.32	Joback Method
cpg	774.89	J/mol×K	976.03	Joback Method
cpg	785.16	J/mol×K	1013.74	Joback Method
dvisc	0.0009535	Pa×s	467.75	Joback Method

dvisc	0.0005512	Pa×s	521.04	Joback Method
dvisc	0.0003528	Pa×s	574.33	Joback Method
dvisc	0.0002435	Pa×s	627.62	Joback Method
dvisc	0.0001782	Pa×s	680.90	Joback Method
dvisc	0.0001364	Pa×s	734.19	Joback Method
dvisc	0.0001083	Pa×s	787.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345745&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