Isophthalic acid, 3,4-dimethylcyclohexyl ethyl ester

Inchi: InChI=1S/C18H24O4/c1-4-21-17(19)14-6-5-7-15(11-14)18(20)22-16-9-8-12(2)13(3)10-16

InchiKey: VOLFDAZXHNGGLK-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CCOC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-255.35	kJ/mol	Joback Method
hf	-665.75	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	76.72	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.845		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	805.69	K	Joback Method
tc	1028.90	K	Joback Method
tf	474.78	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.00	J/mol×K	805.69	Joback Method
cpg	780.94	J/mol×K	842.89	Joback Method
cpg	797.34	J/mol×K	880.09	Joback Method
cpg	812.21	J/mol×K	917.29	Joback Method
cpg	825.56	J/mol×K	954.50	Joback Method
cpg	837.40	J/mol×K	991.70	Joback Method
cpg	847.72	J/mol×K	1028.90	Joback Method
dvisc	0.0009295	Pa×s	474.78	Joback Method

dvisc	0.0005549	Pa×s	529.93	Joback Method
dvisc	0.0003652	Pa×s	585.08	Joback Method
dvisc	0.0002582	Pa×s	640.24	Joback Method
dvisc	0.0001930	Pa×s	695.39	Joback Method
dvisc	0.0001505	Pa×s	750.54	Joback Method
dvisc	0.0001214	Pa×s	805.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343800&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