Isophthalic acid, ethyl neopentyl ester

Inchi: InChI=1S/C15H20O4/c1-5-18-13(16)11-7-6-8-12(9-11)14(17)19-10-15(2,3)4/h6-9H,5,10H
InchiKey: YTOQMVHIFHQPNH-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-286.80	kJ/mol	Joback Method
hf	-626.22	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.066		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
tb	723.61	K	Joback Method
tc	936.77	K	Joback Method
tf	444.49	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.05	J/mol×K	723.61	Joback Method
cpg	611.23	J/mol×K	759.14	Joback Method
cpg	625.36	J/mol×K	794.66	Joback Method
cpg	638.48	J/mol×K	830.19	Joback Method
cpg	650.62	J/mol×K	865.72	Joback Method
cpg	661.80	J/mol×K	901.24	Joback Method
cpg	672.06	J/mol×K	936.77	Joback Method
dvisc	0.0008994	Pa×s	444.49	Joback Method

dvisc	0.0005078	Pa×s	491.01	Joback Method
dvisc	0.0003165	Pa×s	537.53	Joback Method
dvisc	0.0002127	Pa×s	584.05	Joback Method
dvisc	0.0001516	Pa×s	630.57	Joback Method
dvisc	0.0001132	Pa×s	677.09	Joback Method
dvisc	0.0000877	Pa×s	723.61	Joback Method

Sources

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=U343858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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