Isophthalic acid, neopentyl propyl ester

Inchi: InChI=1S/C16H22O4/c1-5-9-19-14(17)12-7-6-8-13(10-12)15(18)20-11-16(2,3)4/h6-8,10H
InchiKey: OYBYREZPPLVSJG-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-278.38	kJ/mol	Joback Method
hf	-646.86	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.456		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	746.49	K	Joback Method
tc	956.97	K	Joback Method
tf	455.76	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.59	J/mol×K	746.49	Joback Method
cpg	666.06	J/mol×K	781.57	Joback Method
cpg	680.47	J/mol×K	816.65	Joback Method
cpg	693.85	J/mol×K	851.73	Joback Method
cpg	706.22	J/mol×K	886.81	Joback Method
cpg	717.63	J/mol×K	921.89	Joback Method
cpg	728.11	J/mol×K	956.97	Joback Method
dvisc	0.0008221	Pa×s	455.76	Joback Method

dvisc	0.0004578	Pa×s	504.22	Joback Method
dvisc	0.0002825	Pa×s	552.67	Joback Method
dvisc	0.0001884	Pa×s	601.12	Joback Method
dvisc	0.0001335	Pa×s	649.58	Joback Method
dvisc	0.0000992	Pa×s	698.03	Joback Method
dvisc	0.0000767	Pa×s	746.49	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=U343859&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