Isophthalic acid, butyl neopentyl ester

Inchi: InChI=1S/C17H24O4/c1-5-6-10-20-15(18)13-8-7-9-14(11-13)16(19)21-12-17(2,3)4/h7-9,
InchiKey: ZMZPTTXSDXYBPT-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.96	kJ/mol	Joback Method
hf	-667.50	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.846		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	769.37	K	Joback Method
tc	977.67	K	Joback Method
tf	467.03	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.20	J/mol×K	769.37	Joback Method
cpg	721.92	J/mol×K	804.09	Joback Method
cpg	736.56	J/mol×K	838.80	Joback Method
cpg	750.15	J/mol×K	873.52	Joback Method
cpg	762.72	J/mol×K	908.23	Joback Method
cpg	774.31	J/mol×K	942.95	Joback Method
cpg	784.95	J/mol×K	977.67	Joback Method
dvisc	0.0007474	Pa×s	467.03	Joback Method

dvisc	0.0004108	Pa×s	517.42	Joback Method
dvisc	0.0002511	Pa×s	567.81	Joback Method
dvisc	0.0001663	Pa×s	618.20	Joback Method
dvisc	0.0001172	Pa×s	668.59	Joback Method
dvisc	0.0000867	Pa×s	718.98	Joback Method
dvisc	0.0000668	Pa×s	769.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343861&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