Isophthalic acid, butyl 3,5-dimethylcyclohexyl ester

Inchi: InChI=1S/C20H28O4/c1-4-5-9-23-19(21)16-7-6-8-17(13-16)20(22)24-18-11-14(2)10-15(3

InchiKey: NEOOEABWSNGRLC-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: CCCCOC(=O)c1cccc(C(=O)OC2CC(C)CC(C)C2)c1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-238.51	kJ/mol	Joback Method
hf	-707.03	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	81.17	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.625		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	851.45	K	Joback Method
tc	1070.31	K	Joback Method
tf	497.32	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.62	J/mol×K	851.45	Joback Method
cpg	898.37	J/mol×K	887.93	Joback Method
cpg	914.53	J/mol×K	924.40	Joback Method
cpg	929.11	J/mol×K	960.88	Joback Method
cpg	942.13	J/mol×K	997.35	Joback Method
cpg	953.60	J/mol×K	1033.83	Joback Method
cpg	963.55	J/mol×K	1070.31	Joback Method
dvisc	0.0007954	Pa×s	497.32	Joback Method

dvisc	0.0004626	Pa×s	556.34	Joback Method
dvisc	0.0002985	Pa×s	615.36	Joback Method
dvisc	0.0002079	Pa×s	674.38	Joback Method
dvisc	0.0001535	Pa×s	733.41	Joback Method
dvisc	0.0001186	Pa×s	792.43	Joback Method
dvisc	0.0000950	Pa×s	851.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343821&Units=SI

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