

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004626	Paxs	556.34	Joback Method
dvisc	0.0002985	Paxs	615.36	Joback Method
dvisc	0.0002079	Paxs	674.38	Joback Method
dvisc	0.0001535	Paxs	733.41	Joback Method
dvisc	0.0001186	Paxs	792.43	Joback Method
dvisc	0.0000950	Paxs	851.45	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

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