

Isophthalic acid, butyl 3-methylphenyl ester

Inchi:	InChI=1S/C19H20O4/c1-3-4-11-22-18(20)15-8-6-9-16(13-15)19(21)23-17-10-5-7-14(2)12
InchiKey:	NTVGPMAHVNZZPY-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-153.18	kJ/mol	Joback Method
hf	-474.97	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.171		Crippen Method
mvol	245.930	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2573.00		NIST Webbook
tb	850.02	K	Joback Method
tc	1076.64	K	Joback Method
tf	526.09	K	Joback Method
vc	0.931	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.25	J/molxK	850.02	Joback Method
cpg	780.85	J/molxK	1038.87	Joback Method
cpg	771.74	J/molxK	1001.10	Joback Method
cpg	761.46	J/molxK	963.33	Joback Method
cpg	749.97	J/molxK	925.56	Joback Method
cpg	737.24	J/molxK	887.79	Joback Method
cpg	788.81	J/molxK	1076.64	Joback Method
dvisc	0.0000652	Paxs	850.02	Joback Method
dvisc	0.0000815	Paxs	796.03	Joback Method

dvisc	0.0001053	Paxs	742.04	Joback Method
dvisc	0.0001415	Paxs	688.06	Joback Method
dvisc	0.0002002	Paxs	634.07	Joback Method
dvisc	0.0003019	Paxs	580.08	Joback Method
dvisc	0.0004955	Paxs	526.09	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=U344517&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

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