

Isophthalic acid, butyl 1-propylbutyl ester

Inchi:	InChI=1S/C19H28O4/c1-4-7-13-22-18(20)15-11-8-12-16(14-15)19(21)23-17(9-5-2)10-6-3
InchiKey:	HSMXLLVMNPBVBFB-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-258.40	kJ/mol	Joback Method
hf	-705.31	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.769		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2201.00		NIST Webbook
tb	817.92	K	Joback Method
tc	1019.49	K	Joback Method
tf	472.15	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.59	J/molxK	817.92	Joback Method
cpg	888.96	J/molxK	985.89	Joback Method
cpg	877.24	J/molxK	952.30	Joback Method
cpg	864.46	J/molxK	918.70	Joback Method
cpg	850.61	J/molxK	885.11	Joback Method
cpg	835.66	J/molxK	851.51	Joback Method
cpg	899.64	J/molxK	1019.49	Joback Method
dvisc	0.0000577	Paxs	817.92	Joback Method
dvisc	0.0000752	Paxs	760.29	Joback Method

dvisc	0.0001024	Paxs	702.66	Joback Method
dvisc	0.0001472	Paxs	645.03	Joback Method
dvisc	0.0002273	Paxs	587.41	Joback Method
dvisc	0.0003857	Paxs	529.78	Joback Method
dvisc	0.0007448	Paxs	472.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U356399&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

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