

Isophthalic acid, butyl 2-methylcyclohexyl ester

Inchi:	InChI=1S/C19H26O4/c1-3-4-12-22-18(20)15-9-7-10-16(13-15)19(21)23-17-11-6-5-8-14(
InchiKey:	BSJJPRYLUFUFLB-UHFFFAOYSA-N
Formula:	C19H26O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-239.22	kJ/mol	Joback Method
hf	-666.05	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.379		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2448.00		NIST Webbook
tb	833.24	K	Joback Method
tc	1054.07	K	Joback Method
tf	490.29	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.77	J/molxK	833.24	Joback Method
cpg	835.20	J/molxK	870.05	Joback Method
cpg	851.12	J/molxK	906.85	Joback Method
cpg	865.54	J/molxK	943.66	Joback Method
cpg	878.48	J/molxK	980.46	Joback Method
cpg	889.97	J/molxK	1017.27	Joback Method
cpg	900.03	J/molxK	1054.07	Joback Method
dvisc	0.0008061	Paxs	490.29	Joback Method
dvisc	0.0004541	Paxs	547.45	Joback Method

dvisc	0.0002851	Paxs	604.61	Joback Method
dvisc	0.0001940	Paxs	661.76	Joback Method
dvisc	0.0001404	Paxs	718.92	Joback Method
dvisc	0.0001065	Paxs	776.08	Joback Method
dvisc	0.0000839	Paxs	833.24	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=U345748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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