Isophthalic acid, butyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H26O4/c1-2-3-12-22-18(20)16-10-7-11-17(13-16)19(21)23-14-15-8-5-4-6-9
InchiKey: CBWNOKNCURZQKJ-UHFFFAOYSA-N
Formula: C19H26O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-231.51	kJ/mol	Joback Method
hf	-645.71	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	79.57	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.381		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2545.00		NIST Webbook
tb	837.91	K	Joback Method
tc	1058.86	K	Joback Method
tf	494.53	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.01	J/mol×K	837.91	Joback Method
cpg	884.72	J/mol×K	1022.03	Joback Method
cpg	873.39	J/mol×K	985.21	Joback Method
cpg	860.68	J/mol×K	948.38	Joback Method
cpg	846.57	J/mol×K	911.56	Joback Method
cpg	831.02	J/mol×K	874.73	Joback Method
cpg	894.70	J/mol×K	1058.86	Joback Method
dvisc	0.0000653	Pa×s	837.91	Joback Method
dvisc	0.0000844	Pa×s	780.68	Joback Method

dvisc	0.0001138	Pa×s	723.45	Joback Method
dvisc	0.0001613	Pa×s	666.22	Joback Method
dvisc	0.0002443	Pa×s	608.99	Joback Method
dvisc	0.0004033	Pa×s	551.76	Joback Method
dvisc	0.0007476	Pa×s	494.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343826&Units=SI
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

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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