

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/molxK	837.91	Joback Method
cpg	831.02	J/molxK	874.73	Joback Method
cpg	846.57	J/molxK	911.56	Joback Method
cpg	860.68	J/molxK	948.38	Joback Method
cpg	873.39	J/molxK	985.21	Joback Method
cpg	884.72	J/molxK	1022.03	Joback Method
cpg	894.70	J/molxK	1058.86	Joback Method
dvisc	0.0007476	Paxs	494.53	Joback Method
dvisc	0.0004033	Paxs	551.76	Joback Method

dvisc	0.0002443	Paxs	608.99	Joback Method
dvisc	0.0001613	Paxs	666.22	Joback Method
dvisc	0.0001138	Paxs	723.45	Joback Method
dvisc	0.0000844	Paxs	780.68	Joback Method
dvisc	0.0000653	Paxs	837.91	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/ci9903071
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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