Isophthalic acid, butyl 3-methylbutyl ester

Inchi: InChI=1S/C17H24O4/c1-4-5-10-20-16(18)14-7-6-8-15(12-14)17(19)21-11-9-13(2)3/h6-8,
InchiKey: DZSILDLXJDNHKX-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-275.24	kJ/mol	Joback Method
hf	-664.03	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.846		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	772.16	K	Joback Method
tc	975.26	K	Joback Method
tf	449.61	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.89	J/mol×K	772.16	Joback Method
cpg	720.52	J/mol×K	806.01	Joback Method
cpg	735.10	J/mol×K	839.86	Joback Method
cpg	748.65	J/mol×K	873.71	Joback Method
cpg	761.19	J/mol×K	907.56	Joback Method
cpg	772.73	J/mol×K	941.41	Joback Method
cpg	783.29	J/mol×K	975.26	Joback Method
dvisc	0.0009014	Pa×s	449.61	Joback Method

dvisc	0.0004783	Pa×s	503.37	Joback Method
dvisc	0.0002868	Pa×s	557.13	Joback Method
dvisc	0.0001882	Pa×s	610.88	Joback Method
dvisc	0.0001322	Pa×s	664.64	Joback Method
dvisc	0.0000979	Pa×s	718.40	Joback Method
dvisc	0.0000756	Pa×s	772.16	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=U356458&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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