

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.89	J/molxK	772.16	Joback Method
cpg	772.73	J/molxK	941.41	Joback Method
cpg	761.19	J/molxK	907.56	Joback Method
cpg	748.65	J/molxK	873.71	Joback Method
cpg	735.10	J/molxK	839.86	Joback Method
cpg	720.52	J/molxK	806.01	Joback Method
cpg	783.29	J/molxK	975.26	Joback Method
dvisc	0.0000756	Paxs	772.16	Joback Method

dvisc	0.0000979	Paxs	718.40	Joback Method
dvisc	0.0001322	Paxs	664.64	Joback Method
dvisc	0.0001882	Paxs	610.88	Joback Method
dvisc	0.0002868	Paxs	557.13	Joback Method
dvisc	0.0004783	Paxs	503.37	Joback Method
dvisc	0.0009014	Paxs	449.61	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=U356458&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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