

Phthalic acid, butyl 3,3-dimethylbut-2-yl ester

Inchi:	InChI=1S/C18H26O4/c1-6-7-12-21-16(19)14-10-8-9-11-15(14)17(20)22-13(2)18(3,4)5/h8
InchiKey:	SIQIRVRXKIPZPY-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-263.98	kJ/mol	Joback Method
hf	-693.42	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.235		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinsol	2029.00		NIST Webbook
tb	791.81	K	Joback Method
tc	1001.25	K	Joback Method
tf	463.30	K	Joback Method
vc	0.967	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.36	J/molxK	791.81	Joback Method
cpg	779.50	J/molxK	826.72	Joback Method
cpg	794.50	J/molxK	861.62	Joback Method
cpg	808.40	J/molxK	896.53	Joback Method
cpg	821.22	J/molxK	931.44	Joback Method
cpg	833.02	J/molxK	966.34	Joback Method
cpg	843.81	J/molxK	1001.25	Joback Method
dvisc	0.0007844	Paxs	463.30	Joback Method
dvisc	0.0003954	Paxs	518.05	Joback Method

dvisc	0.0002272	Paxs	572.80	Joback Method
dvisc	0.0001438	Paxs	627.55	Joback Method
dvisc	0.0000980	Paxs	682.31	Joback Method
dvisc	0.0000707	Paxs	737.06	Joback Method
dvisc	0.0000533	Paxs	791.81	Joback Method

Sources

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=U357002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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