Terephthalic acid, butyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C18H26O4/c1-5-6-11-21-17(19)15-7-9-16(10-8-15)18(20)22-14(4)12-13(2)3/h7

InchiKey: MFZTXUTYTBVJIN-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CCCCOC(=O)c1ccc(C(=O)OC(C)CC(C)C)cc1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-269.26	kJ/mol	Joback Method
hf	-689.95	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.235		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	794.60	K	Joback Method
tc	999.14	K	Joback Method
tf	445.88	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.32	J/mol×K	794.60	Joback Method
cpg	831.61	J/mol×K	965.05	Joback Method
cpg	819.91	J/mol×K	930.96	Joback Method
cpg	807.15	J/mol×K	896.87	Joback Method
cpg	793.31	J/mol×K	862.78	Joback Method
cpg	778.37	J/mol×K	828.69	Joback Method
cpg	842.26	J/mol×K	999.14	Joback Method
dvisc	0.0000608	Pa×s	794.60	Joback Method

dvisc	0.0000803	Pa×s	736.48	Joback Method
dvisc	0.0001112	Pa×s	678.36	Joback Method
dvisc	0.0001637	Pa×s	620.24	Joback Method
dvisc	0.0002611	Pa×s	562.12	Joback Method
dvisc	0.0004637	Pa×s	504.00	Joback Method
dvisc	0.0009566	Pa×s	445.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356257&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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