Phthalic acid, isobutyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C18H26O4/c1-6-16(13(4)5)22-18(20)15-10-8-7-9-14(15)17(19)21-11-12(2)3/h7
InchiKey: YYUSAGVQOPKRBV-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCC(OC(=O)c1ccccc1C(=O)OCC(C)C)C(C)C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-695.23	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.091		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	794.16	K	Joback Method
tc	1001.35	K	Joback Method
tf	430.88	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.86	J/mol×K	794.16	Joback Method
cpg	779.12	J/mol×K	828.69	Joback Method
cpg	794.22	J/mol×K	863.22	Joback Method
cpg	808.19	J/mol×K	897.75	Joback Method
cpg	821.04	J/mol×K	932.29	Joback Method
cpg	832.78	J/mol×K	966.82	Joback Method
cpg	843.45	J/mol×K	1001.35	Joback Method
dvisc	0.0011366	Pa×s	430.88	Joback Method

dvisc	0.0005049	Pa×s	491.43	Joback Method
dvisc	0.0002680	Pa×s	551.97	Joback Method
dvisc	0.0001612	Pa×s	612.52	Joback Method
dvisc	0.0001063	Pa×s	673.07	Joback Method
dvisc	0.0000751	Pa×s	733.61	Joback Method
dvisc	0.0000559	Pa×s	794.16	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=U356907&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